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CALCULATION OF THE LOWEST ENERGY STATE OF THE CONDUCTION BAND OF GOLD

WALTER J. SLAZAK
and
FRANCESCO MUSORRAFITI

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and

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by

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Submitted in partial fulfillment of
the requirements for the degree of

MASTER OF SCIENCE
IN
PHYSICS

United States Naval Postgraduate School
Monterey, California

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ABSTRACT

A new central field potential was developed for the metal gold by a variational technique in conjunction with the Wigner Seitz cellular method using the Control Data 1604 Computer to perform the calculations. The Hartree potential for the Au^{+} ion was used as a starting point of the variations. The first variation was made fixing one point of the Hartree potential and letting the shape of the potential curve vary arbitrarily. The particular potential was chosen which furnished the lowest energy state solution to the Schroedinger radial wave equation subject to the boundary condition that the solution also furnished the proper ionization energy. A second variation was made varying the initially selected fixed point. This variation was terminated when the solution furnished the accepted value of the atomic radius, 1.59 Angstrom units. The results of the calculation indicate a lowest energy state of 1.194 Rydbergs and a cohesive energy of 81.6 kilogram calories per mole which compares favorably to the accepted value 83.5 kilogram calories per mole.

The wave functions from the developed potential indicate that the exchange interaction between the outer electrons are a major contribution to the cohesive energy.

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INTRODUCTION

The original scope of the thesis was to determine the lowest energy state of the conduction band of gold employing the cellular method, using a known tabulated potential.

The investigation progressed in five distinct phases.

The initial efforts were mainly along classic lines. A program was developed to use the Control Data 1604 Computer as a tool to make the computations. The initial results looked very promising. A method was devised to make a complete Wigner-Seitz (W-S) cellular calculation with one program. Work had begun to include correlation and exchange interactions. The Thomas Fermi potential was used in these initial investigations. The results for copper, even though they did not agree with the accepted values, seemed to agree with what had been done by others. Wave functions and W-S calculations were made for about twenty metals and carefully cataloged, with the aim that as the methods developed for gold the calculations could be repeated for other metals.

The second phase was a phase of great distress. By this time a very great number of calculations had been made and it was observed that the results were not consistent. Different intervals, changes of scale during calculation and different computational methods gave different results. At this point the exact cause of problem was unknown. Possible causes were estimated to be: improper programming, machine malfunctioning, input data too crude, inadequacy of numerical computational methods, or invalidity of the Wigner-Seitz cellular method. In any case except for an invalid program or improper machine operation, the problem area was one of far-reaching consequences. Standard computation methods had been used and

if these methods were at fault there would be implications that all computations to date were nonsense. If the cellular method did not converge, then too all the computations to date would have to be discarded.

The third phase was spent in isolating and resolving the problem area. This was accomplished in the following manner. The test vehicle used was the calculation of the wave functions of sodium as in the original Wigner-Seitz paper.[1] The potential used in this calculation was the Prokofiev ion core potential. This potential is represented by a series of parabolas, therefore there was no problem of fitting points to any interval. A unique method of solving the Schroedinger Differential Equation was devised based on an extension of Boole's Operational Methods.[2] In essence the method consisted of solving the entire problem in steps as a series of boundary value problems, requiring convergence at each step. The original Wigner-Seitz Data[1] was duplicated using this method. It was also found that a simple difference formula at one one-hundredth Bohr unit interval also duplicated the data. The results of the investigation confirmed the validity of the Wigner-Seitz method and provide a tool to continue the calculations. The investigation also indicated that predictor corrector type calculations in general as well as interval changes during a calculation led to erroneous results and were useless for this work. All previous work to this date had to be discarded.

---

[1] E. Wigner and F. Seitz, Phys. Rev. 43, 804(1933) and Phy. Rev. 46, 509(1934).

[2] G. Boole, Treatise on Differential Equations, Supplementary Volume (The University Press, Cambridge, 1865) Chapter XXX.

The fourth phase was to use the method as developed on existing potentials of the noble metals. The results were disappointing and were not as good as the previous erroneous calculations. One striking physical fact was noted. When the method was applied to sodium using the ionization energy in the calculation the proper form of the wave functions resulted. All of the potentials of the noble metals investigated represented an ionization energy that was appreciably lower than the accepted value.

The fifth and final phase was used to develop a new metallic gold potential. The question was posed: could a variational technique be used to find a potential which gave the proper ionization energy and possibly give a lowest energy state? This idea was based on the assumption that such a potential would be more than a bare ion core potential, but would include exchange, correlation and proper electron screening constants. The calculation proved successful using the computation procedures already established as above. A potential was devised which gives in the Wigner-Seitz cellular calculation for gold the accepted values of the atomic radius and cohesive energy.

MATHEMATICAL AND PHYSICAL BACKGROUND

The Cohesive Energy

The cohesive energy[3] is defined as "the difference between the energy of a crystal in the normal bound state at absolute zero of temperature, and the energy of the isolated atoms or molecules of which it is composed."

The cohesive energy is discussed first in order to introduce the total contributions to the energy of a solid. A rather complete list of contributions to the cohesive energy is quoted from Jaswon[4] . . . .

> . . . . . the total electronic energy of a solid may be regarded as the sum of three distinct contributions:-
>
> 1. The energy associated with the ion-cores, viz.
>   (a) the self-energies of the ion-cores. This is independent of interatomic distance until the closed shells begin to overlap, and hence does not enter into the calculation of the equilibrium lattice parameter and compressibility;
>   (b) the Coulomb interaction of the ion-cores;
>   (c) the exchange interaction of the ion-cores. This is not important in the alkalis owing to the large clearance between the ions, but it assumes greather importance for the noble metals--especially in determining the elastic constants;
>   (d) the Van der Waals interaction energy of the ion-cores. This is taken to be negligible for all except molecular solids and graphite, but may be a contributory factor in the high cohesion of the transition elements.
> 2. The energy associated with the valence electrons, viz.
>   (a) the kinetic energy;
>   (b) the potential energy (with respect to the field of the ion-cores);
>   (c) the Coulomb self-potential;

---

[3] F. Seitz, The Modern Theory of Solids (McGraw Hill Book Co., Inc., New York, 1940), p. 375.

[4] M. A. Jaswon, The Theory of Cohesion (Interscience Publishers, Inc., New York, 1954), p.p. 156, 157.

(d) the exchange interaction energy. This may be regarded as a correction to (c) operative for electrons of parallel spin;

(e) the correction to (c) for electrons of anti-parallel spin. This is not included in the mean value $\overline{H}$ of the Hamiltonian of the solid, and has to be estimated independently.

3. The interaction between the valence and ion core electrons, viz.
   (a) the Coulomb interaction. This has already been accounted for by 2(b);
   (b) the exchange and correlation interactions.

The Cellular Method

The cellular method is discussed in great detail in many standard works in solid state physics. In this paper only those portions of the cellular method which pertain to the problem at hand will be discussed.

Consider a face centered cubic crystal and consider the construction of a cell obtained by choosing one ion core as a center and then passing planes perpendicular to and at the midpoint of the lines between the chosen ion center and all other nearest neighbors. The result is a polyhedron known as the "Wigner-Seitz Cell." This polyhedron to a first approximation may be considered a spherical cell.

For a face centered cubic crystal the radius of this approximating sphere can be calculated equating the volume of the cell per electron to volume of the lattice per electron.

$$\frac{4\pi r_0^3}{3} = \frac{A_0^3}{4} \qquad r_0^3 = \frac{3A_0^3}{16\pi} \qquad r_0 = A_0(3/16\pi)^{1/3}$$

$r_0 =$ radius of sphere

$A_0 =$ edge length of the fundamental cube of a cubic lattice

Values of r_0 are indicated in Table I for copper, silver, and gold.

The Wigner Seitz Cellular Approximation[5]

The original work was accomplished for metallic sodium and is reviewed in some detail; first, in that the method was used in this thesis, secondly, the results of the calculations for the metal dosium were unusually close to the accepted values, and thirdly there is a difference in interpretation as to the constitution of the potential used.

The argument is that the polyhedral cell can to a first approximation be replaced by a spherical cell. An ion core potential was considered inside the cell, with the condition this potential was spherically symmetric or could be averaged out to be spherically symmetric. The basic Schroedinger equation becomes a radial wave equation in this case in the form:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(r) = E\,\psi(r)$$

introducing $\psi(r) = rR(r)$ the equation becomes

$$\frac{d^2R(r)}{dr^2} - \frac{2m}{\hbar}\left[V(r) - E\right]R(r) = 0$$

Introducing natural units

1 Bohr radius = .529 Angstrom Units = $a_0 = \dfrac{\hbar^2}{4\pi^2 m e^2}$

1 Rydberg = 13.5 electron volts = $\dfrac{e^2}{2a_0}$

The equation becomes

$$\frac{d^2R(r)}{dr^2} - \left[2\;V(r)\quad E\right]R(r) = 0$$

with E in Rydbergs

r in Bohr radii

---

[5] E. Wigner and F. Seitz, Phys. Rev. 43, 804(1933)

TABLE I

Values of the Edge Length of the Fundamental Cube for Cubic Lattices (A_o) and the Atomic Radius (r_o) for Gold, Silver, and Copper.

	Gold	Silver	Copper
A_o = [a](Angstrom Units)	4.070	4.078	3.609
r_o = (Angstrom Units)	1.59	1.59	1.41
r_o = (Bohr Units)	3.01	3.01	2.67

1 Bohr Unit = .529 Angstrom Unit

---

[a] F. Seitz, The Modern Theory of Solids, op. cit. p. 6

The boundary condition inherent in the cellular method required by the periodicity of the lattice structure and symmetry is that the derivative of the wave function in the direction perpendicular to the symmetry planes will be zero when evaluated at the plane. When the polyhedron is approximated to a sphere the boundary condition becomes

$$\frac{d\psi(r)}{dr} = 0 \quad \text{OR} \quad \frac{\partial R(r)}{\partial r} = \frac{R(r)}{r} \qquad \text{WHERE} \quad rR(r) = \psi(r)$$

It was further assumed that the electrons outside the cell boundary represented a free electron gas and that the average energy per electron could be represented by the Fermi energy

$$\epsilon_f(r_0) = \frac{3\hbar^2}{10m^2}\left(\frac{3N}{8\pi}\cdot\frac{3}{N4\pi r_0^3}\right)^{2/3} = \frac{2.21}{r_0^2} \ \text{RYDBERGS}$$

$\hbar$ = Plancks constant

m = mass of the electron

N = number of electrons per unit volume

r_0 = atomic radius (or radius of cell)

The potential used in the calculation was the Prokofiev ion core potential for sodium.[6] This choice of potential was fortuitous in many respects as follows:

1. The potential was obtained from actual data.

2. The potential was represented by a series of parabolas instead of just a number of points, thus the value of the potential at any value of could be determined accurately.

---

[6] E. V. Condon and G. H. Shortley, The Theory of Atomic Spectra (Cambridge University Press, London, 1951), p.343.

3. Within the first 1/100 interval, the potential is a constant. Therefore an initial power series expansion around the origin is valid. This initial power series expansion is required to furnish starting values for the wave function calculations by iterative processes.

The most important and striking feature of the potential is that when the radial wave equation is solved using the ionization energy for E, the resulting wave equations approach zero as r approaches infinity. Thus this potential actually represents the ionization energy and is physically much more than a simple ion core potential. Included within the potential are exchange, electron-electron and ion-ion contributions. This interpretation may be disagreed with on the grounds that non-central fields would be represented by central fields if the interpretation was correct. Actually the interpretation given implies that the contributions to the potential are smeared out in the spherical symmetry approximation. Also - since the results were close to the accepted values, it appears that there is more involved than the coincidence of various contributions cancelling each other. The contributions may actually be physically present in the potential. The results also indicate that the spherical symmetric model is a very good model for sodium.

The equation $\frac{d^2R(r)}{dr^2} - 2\left[V(r) - E\right] R(r) = 0$

was solved for different values of the energy. Curve 1 of Fig. 1 represents the radial wave function when E is equal to the ionization energy. Curve 2 represents the radial wave function for a higher energy. The boundary condition $\frac{\partial R(r)}{\partial r} = \frac{R(r)}{r}$ is met at two points on Curve 2. This boundary condition is met only at one point on Curve 3, and not at all for higher values of E.

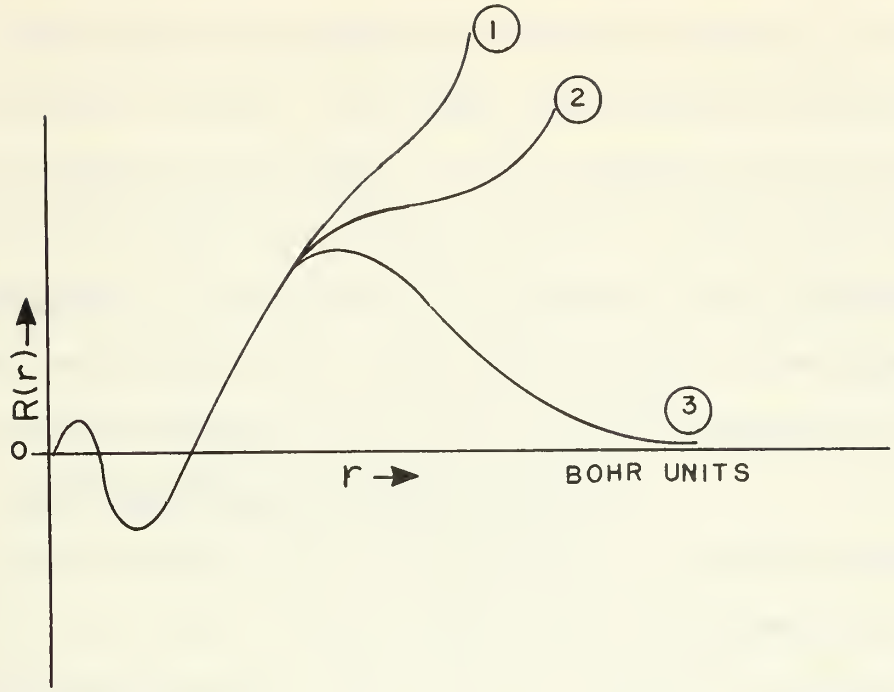

Fig. 1. Plot of the Radial Wave Functions R(r) vs. Radial Distance (r) for a Wigner Seitz Cellular Calculation of a Metal. The wave function ① represents the ionization energy. The wave function ③ represents the lowest energy state.

The values of E satisfying the boundary conditions are plotted vs. r as in Curve 1 in Fig. 2. The lowest energy state is that point determined by the curve with one tangent. Curve 2 represents the total energy and includes the addition of the Fermi energy for a free electron gas. The atomic radius, or the radius of the spherical cell is indicated by the lowest point on this curve. The cohesive energy is the difference between the ionization energy and the value of Curve 2 evaluated at r_o.

The Thomas-Fermi Universal Potential[7,8]

This potential which is represented by a tabulated function can be scaled to any value of Z the atomic number. The Thomas-Fermi potential is an approximate central field potential, obtained by treating a cluster of electrons around a nucleus by Fermi Dirac Statistics.

$$V(r) = \frac{Ze}{r}\phi(x)$$

$$r = bx$$

$$b = \frac{1}{2}\left(\frac{3\pi}{4}\right)^{2/3} \cdot \frac{a_o}{Z^{1/3}} = \frac{.88534\, a_o}{Z^{1/3}}$$

$\phi(x)$ is a tabulated function

Z = atomic number

r = radius in Bohr units

a_o = 1 Bohr radius = .529 Angstrom units

e = Charge on the electron

---

[7] H. J. Brudner, A Thomas-Fermi Technique for Determining Characteristics of Alkali Atoms with Excited Valence Electrons (New York University, College of Engineering, prepared for The Office of Naval Research, Physics Branch, Washington, D.C., 1959) and Accurate Thomas-Fermi Potential Distributions for the Alkali Ions (New York University, College of Engineering, Research Div., prepared for The Office of Naval Research, Physics Branch, Washington, D.C., 1959, Contract No. ONR 285(15)).

[8] E. V. Condon and G. H. Shortley, op. cit., p. 337.

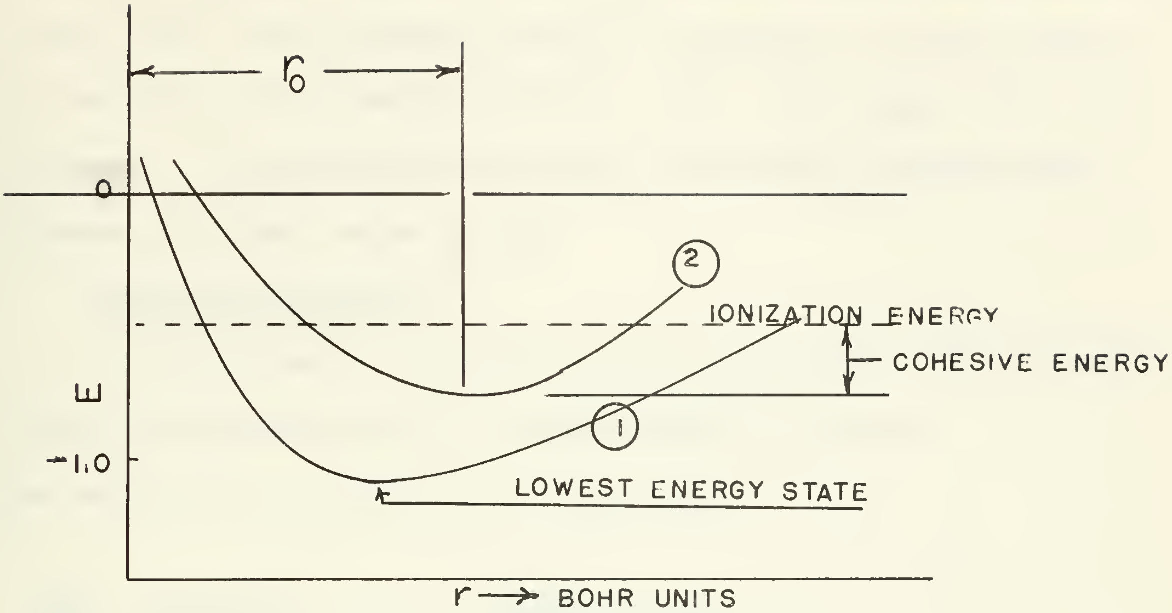

Fig. 2. Plot of the Energy (E in Rydbergs) vs. the Radial Distance (r_o in Bohr units) for Values of the Wave Function R(r), Satisfying the Boundary Condition:

$$\frac{\partial R(r)}{\partial r} = \frac{R(r)}{r}$$

Curve 1 portrays the fundamental relation. The lowest value of energy on Curve 1 represents the lowest energy state. Curve 2 is obtained from Curve 1 by the addition of the Fermi Energy. The value of r at the minimum of Curve 2 represents the atomic radius. The energy difference between the ionization energy and the minimum of Curve 2 represents the cohesive energy.

A partial table of $\phi(X)$ for the free atom is found in Condon and Shortley.[9] Brudner[10] gives values of the Thomas-Fermi potential for the alkali ions. It was observed that the ion potential for the cesium ion corresponded to the free atom potential except near large values of the argument X. These functions are given at one-tenth intervals of the argument X and were easier to use.

The Hartree Potential

A brief discussion of the terms used in the Hartree self consistent field is described herein for equations without exchange.

The equation for the radial wave function is

$$\frac{d^2R}{dr^2} = \frac{2Y(n,\ell,r)}{r} - \epsilon_{n,\ell} - \frac{\ell(\ell+1)}{r^2} P(n,\ell,r) = 0$$

$\frac{Y(n,\ell,r)}{r}$ is the potential of the field of the nucleus and of the average distribution of the electrons.

$P(n,\ell,r)$ is the radial wave function, n,ℓ is a description of the state.

The field at radius r due to the charge on the nucleus and the average distribution of the electrons is $\frac{Z(r)}{r^2}$

$Z(r)$ is related to $Y(r)$ by the relations

$$\frac{dY(r)}{dr} = \frac{1}{r}\left[Y(r) - Z(r)\right]$$

or

$$\frac{d}{dr}\left[\frac{Y(r)}{r}\right] = -\frac{Z(r)}{r^2}$$

---

[9] E. V. Condon and G. H. Shortley, op. cit.

[10] H. J. Brudner, op, cit.

In the case of silver,[11] the values of Y(r) are tabulated. In the cases of copper[12] and gold,[13] the contributions to Z(r) are given and Y(r) is calculated by use of the above equations.

---

[11] M. M. Black, Memoirs and Proceedings of the Manchester Lit. and Phil. Soc., v. 79, 1934-35.

[12] D. R. Hartree, Proc. Roy. Soc., London, A 141,282 (1933).

[13] A. S. Douglas and D. R. Hartree, Proc. Roy. Soc., London (1934).

CALCULATION

The Initial Approach

The initial approach used the Thomas-Fermi potential in the calculation. The aim of the initial approach was to establish the program for the Control Data 1604 Computer to give results from which graphs like Fig. 1 and Fig. 2 could be plotted.

In dimensionless form the radial wave equation took the form

$$\frac{d^2R}{dx^2} + \left[1.7706\, Z^{2/3}\frac{\emptyset(x)}{x} - \frac{1.571\, E}{Z^{2/3}}\right] R = 0$$

Z is the atomic number

E is the energy in units of two Rydbergs

$\emptyset(x)$ is the Thomas-Fermi tabulated function

A simple difference equation solution was adopted[14] as follows:

Let $$f(x) = 1.7706\, Z^{2/3}\frac{\emptyset(x)}{x} - \frac{1.571\, E}{Z^{2/3}}$$

$$R(x+\Delta x) = \left\{2 - (\delta x)^2 f(x)\right\} R(x) - R(x-\Delta x)$$

The program was successfully developed. A format was established using r in Bohr units as independent variable instead of X. In this format a contribution to the effective potential normalized to $1/Z$ could be inserted on data cards, changing only Z and the ionization energy for different elements.

That is $V(r) = \dfrac{Z\emptyset(r)}{r}$

---

[14] J. C. Slater, Mechanics (McGraw Hill Book Co., Inc., 1947), Appendix I.

Difficulties Experienced

In order to insure the most accurate calculation having established the format of the program, iterative methods reputed to be more accurate than the initial simple iterative formula were tried. The Milne[15] fifth and seventh degree polynomial methods for second degree differential equations without a first order term were representative of accurate predictor-corrector type formulae.

It was observed that using the same potential that different numerical formulae gave different solutions. It was also noted that changing scale, or changing intervals during the course of the solution also gave different results.

Another major problem area developed, how to interpolate data. Much of the tabulated data is given to only two decimal places. This type of data to a machine that sees 12-100 decimal places appears as a widely scattered set of points. That is, the problem area was how sensitive are the various iterative formulae to crude data.

The basic form of the equation

$$\frac{d^2R}{dr^2} = f(r) \cdot R$$

tends to become unstable[16] for large values of r. The question arose, did spurious solutions which were originally eliminated by the boundary conditions creep back during the calculation?

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[15] W. E. Milne, Numerical Calculus (Princeton University Press, 1949), p.p. 140-143.

[16] L. Fox, Numerical Solutions of Ordinary and Partial Differential Equations (Addison-Wesley Publishing Co., Inc., London, 1962) p.p. 46-57.

Investigation of the Problem Areas

The next basic step was to determine if the Wigner Seitz method was actually convergent, and if so, what scheme of calculation was required with the tools on hand to give a proper solution.

The vehicle for the investigation was the use of the Prokofiev potential to make a calculation for E equal to .5 Rydbergs. A plot of this function was available in the literature.[17] At this energy there were two tangents to the curve. Since the Prokofiev potential is a series of parabolas the values of the function are readily calculated to any desired degree of accuracy by the computer. This potential eliminated one variable, scatter in the data.

The interval chosen was 1/100 of a Bohr radius. Choosing a fixed interval eliminated another variable.

A new scheme was developed to solve the basic equation based on Boole's operational methods.[18] A sketch of the method follows; full details are in Appendix I.

The first three points of the potential are approximated by a parabola. The radial wave equation is then solved in the interval of these three points. The value of the function and the derivative are then evaluated at midrange. The process is then repeated for the second, third, and fourth points, using the previous calculated values of the function and derivative as initial conditions. Thus in the range of 830 points the

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[17] E. Wigner and F. Seitz, Phys. Rev. 43, 804 (1933)

[18] G. Boole, Treatise on Differential Equations, Supplementary Volume (The University Press, Cambridge, 1865), Chapter XXX

process is simply the solution of 829 boundary value problems. The solution turned out to be a very complex series solution, which converged at every interval. The length and complexity of the solution were initially disappointing in that one run required approximately twenty minutes of machine time, and would require a lifetime for one man to accomplish by ordinary calculation processes.

The Resolution of the Problem

The second derivative of R(r) can be determined by two methods from the solution R(r) as follows:

1. $\frac{d^2R}{dr^2} = f(r) \cdot R(r)$ the original equation.

2. Differentiate the function R(r) twice with respect to r.

The values of the second derivative calculated by both of the above methods must match for the equations to be consistent.

The Radial Wave Functions R(r) were calculated for sodium for the energy state, E = 0.5 Rydbergs by a variety of computational techniques including the boundary value method, the simple type difference method, and predictor-corrector methods.

The wave functions were then compared with the Wigner-Seitz wave function with surprising results. A summary of the results follows:

1. The boundary value technique proved successful. The values of the two second derivatives matched within 10^{-8}. The wave function matched the Wigner-Seitz function from the literature point by point.

2. The simple system after some small initial perturbations matched the solution calculated by the boundary value method within 10^{-6} for the function, the first derivative and the second derivative.

3. The predictor-corrector formulae gave varied results and did not

duplicate the Wigner-Seitz wave function. It was observed that this method of solution in matching the second derivative and holding the function could not hold the first derivative. The net result is that the first derivative was not continuous from point to point. The second derivative obtained by differentiating the first derivative turned out to be a series of widely varying oscillations.

4. In Fig. 3 the wave function calculated by the boundary value method and the simple method coincide with the wave function from the literature. The predictor-corrector method carried to three decimal places (duplicating hand calculation) differed greatly from the same method carried to five or one hundred decimal places.

The Criteria Established

The following criteria were established as a result of the investigation:

1. The simple method was adopted using the 1/100 Bohr Unit interval without any change in scale during the calculation.

2. The boundary value method would be used to obtain accurate starting values for the simple method.

3. Extreme care would have to be exercised in the data points used. The potential curves used were expanded graphically to insure that spurious "wiggles" were not introduced.

Conclusions

The problem had been resolved and it was concluded.

1. The Wigner-Seitz cellular method does converge, but much care must be used in the calculations as the many pitfalls along the way can lead to erroneous results which are not obviously erroneous.

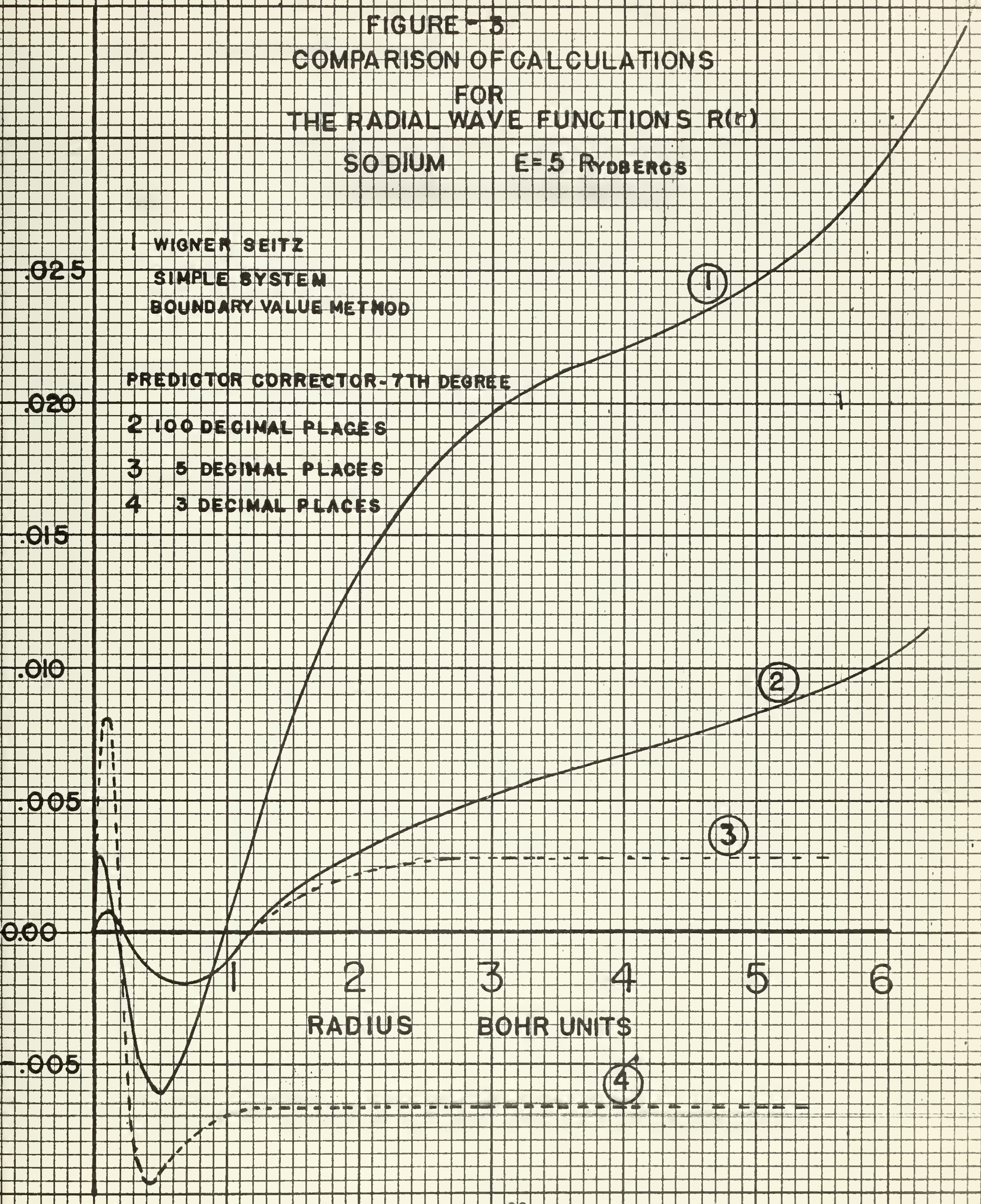

FIGURE - 3
COMPARISON OF CALCULATIONS
FOR
THE RADIAL WAVE FUNCTIONS R(r)
SODIUM E=.5 RYDBERGS

2. The calculations would be carried out using the above mentioned criteria without further refinement.

WIGNER-SEITZ CALCULATIONS FOR THE NOBLE METALS USING EXISTING POTENTIALS

The Potentials Used

The Hartree silver potential[19] and the Thomas-Fermi potential are compared in Fig. 4 on a log-log plot. It is observed there is rather close agreement between the two potentials. The Thomas-Fermi free atom potential was arbitrarily fitted into the Hartree potential for large values of r so that the Thomas-Fermi potential would resemble an ion core potential.

The Hartree Fock copper potential[20] and the Thomas-Fermi copper potential are compared on a log-log plot in Fig. 5. The Hartree potential is not shown as it agrees fairly well with the Thomas-Fermi potential.

The Hartree gold potential[21] and the Thomas-Fermi gold potential are compared on a log-log plot in Fig. 6. It is again noted that there is rather good agreement.

The wave functions for the noble metals employing the six potentials discussed above are graphically portrayed in Figs. 29 through 75 (See Appendix II) for the range of energies varying from the ionization energy to the lowest energy state. These graphs are depicted as obtained from the computer graph routine without retouching.

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[19] M. M. Black, op. cit.

[20] G. W. Pratt, Phys. Rev., 88, 1217 (1952).

[21] A. S. Douglas and D. R. Hartree, op. cit.

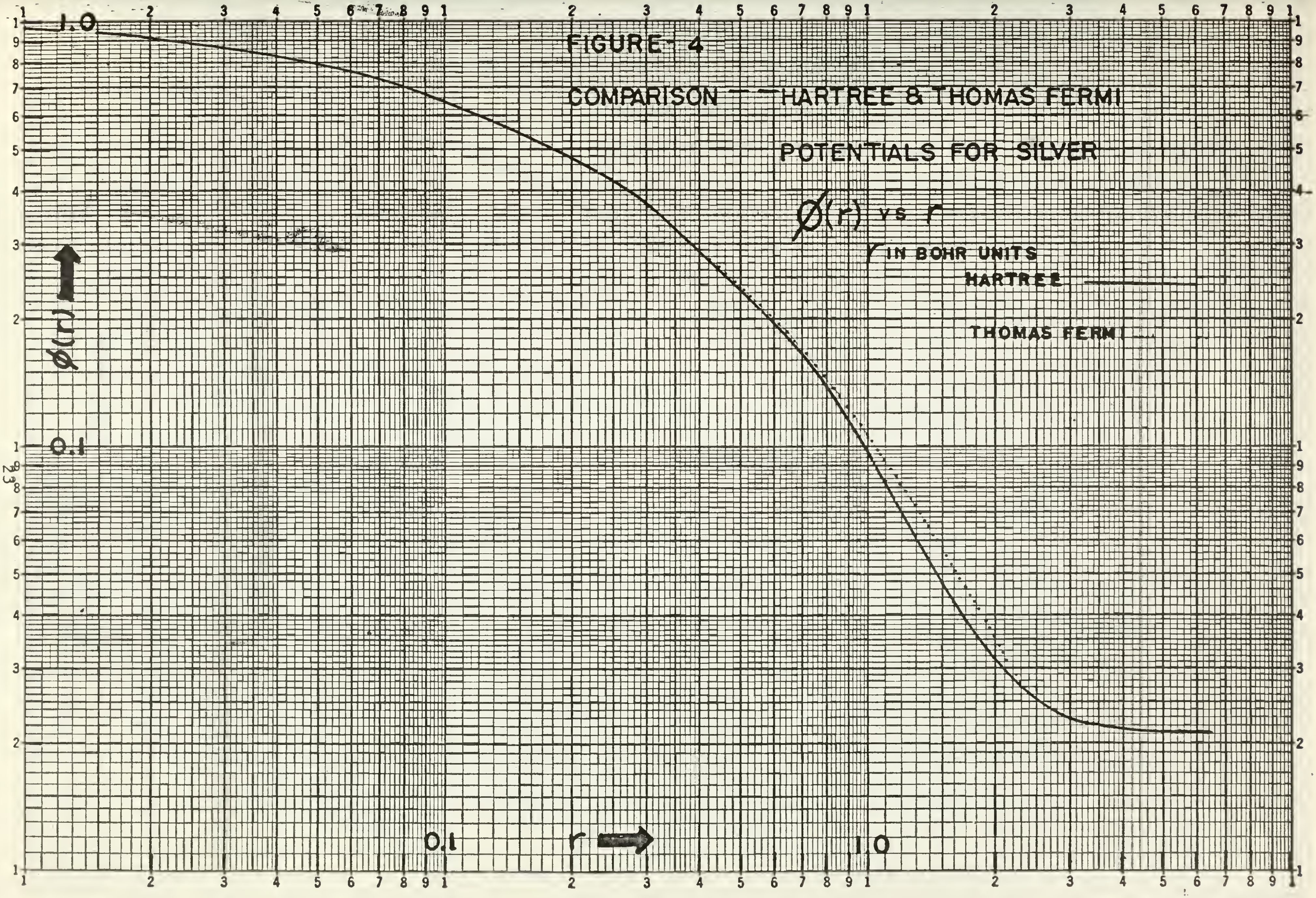

FIGURE 4

COMPARISON — HARTREE & THOMAS FERMI

POTENTIALS FOR SILVER

K&E LOGARITHMIC 358-112
KEUFFEL & ESSER CO. MADE IN U.S.A.
2 X 3 CYCLES

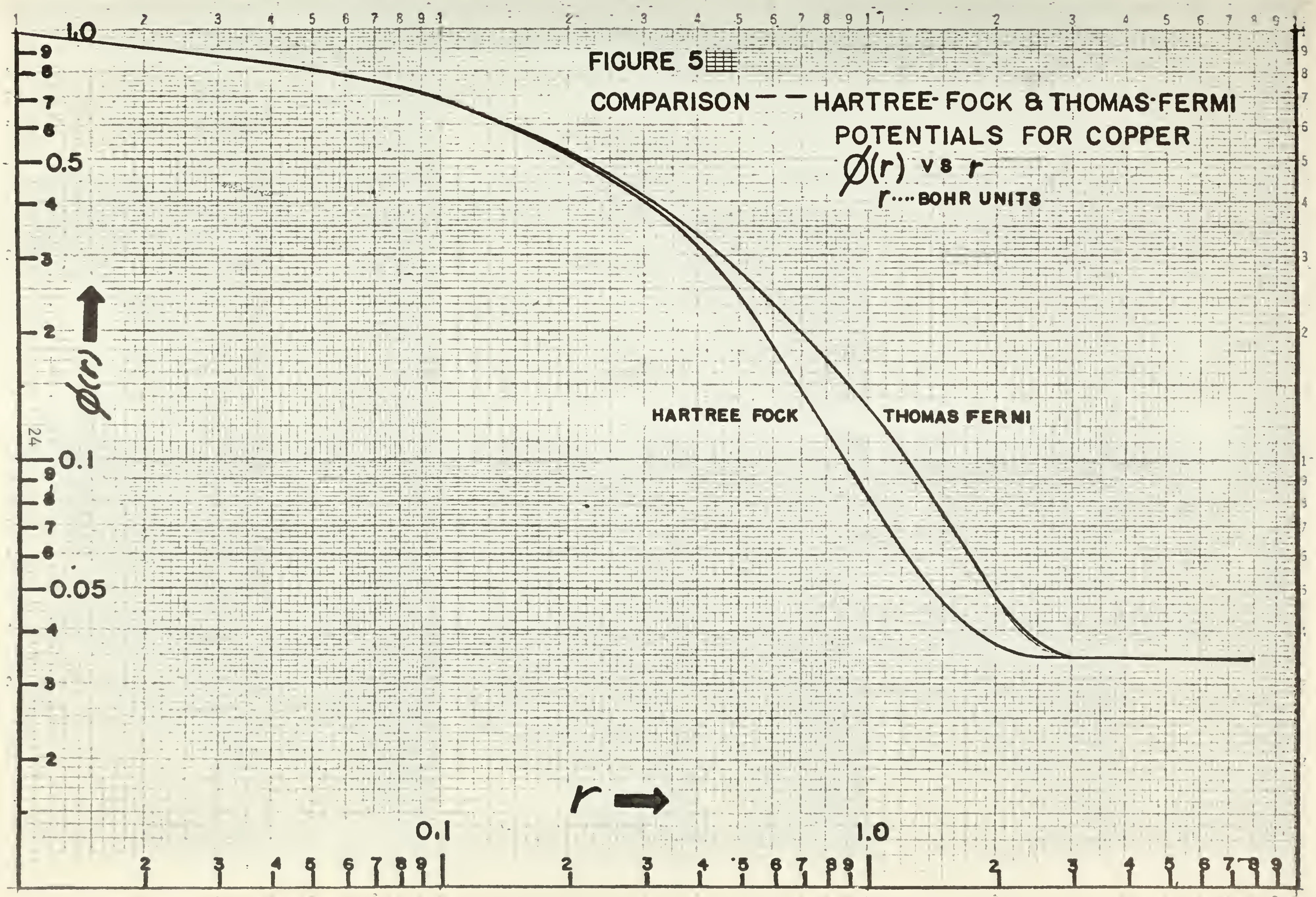

FIGURE 5

COMPARISON — HARTREE-FOCK & THOMAS-FERMI POTENTIALS FOR COPPER

$\phi(r)$ vs r

r.... BOHR UNITS

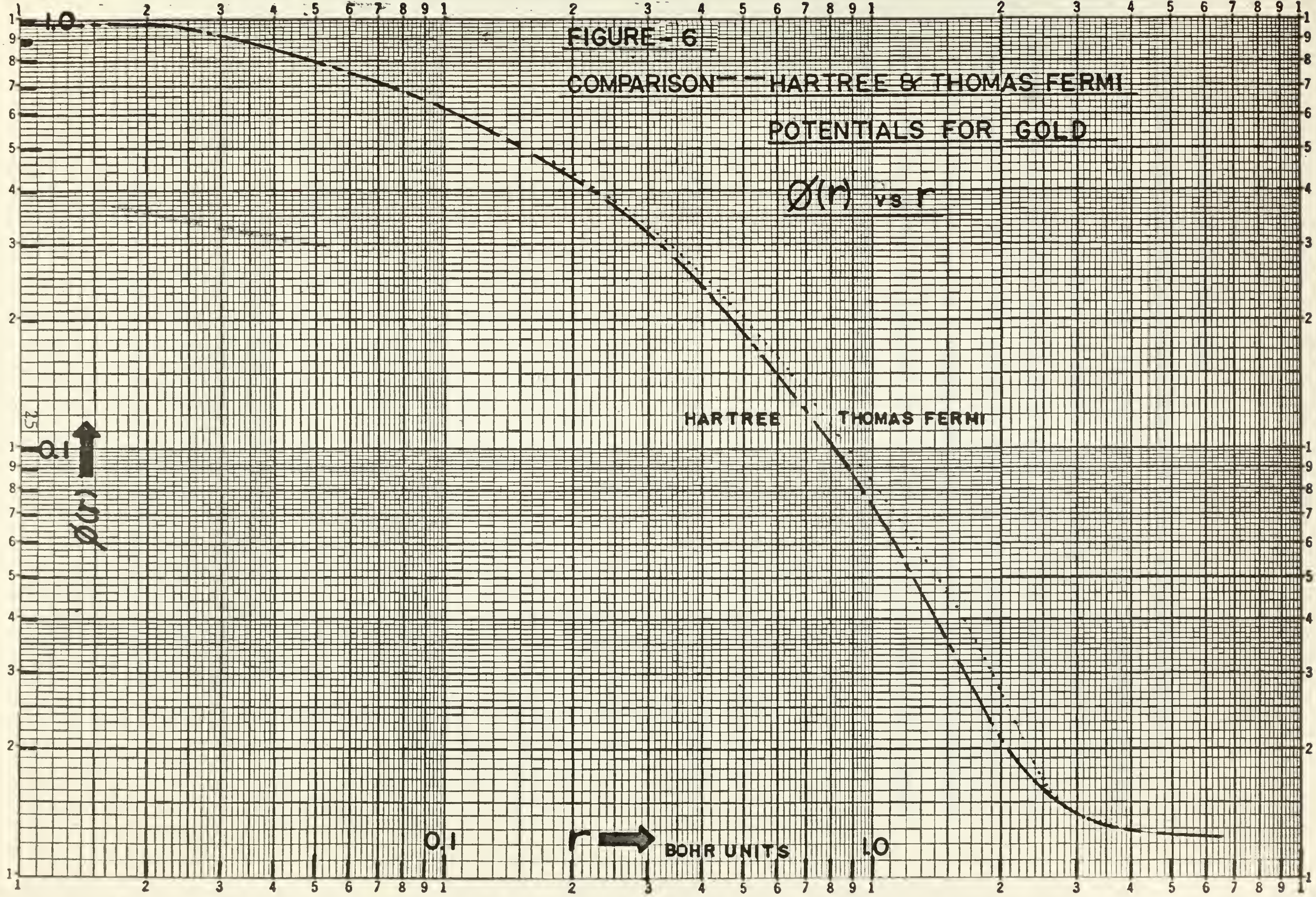

FIGURE - 6

COMPARISON — HARTREE & THOMAS FERMI POTENTIALS FOR GOLD

$\phi(r)$ vs r

Comparison of Calculations

Tables II and III summarize the results of the calculations.

The results were rather surprising, none of the potentials actually represented the ionization of energy. The Thomas-Fermi copper is the nearest to representing an accepted value (80%). The Hartree gold potential represented 52% of the accepted value of the ionization energy.

These results may be a strong indication that the ion core potential of a free ion should be replaced by a potential more suitable for a metal rather than corrections be made to the free ion potential.

TABLE II

Comparison of Calculations and Accepted Values for the Lowest Energy State and Atomic Radius of Copper, Silver, and Gold.

	Lowest Energy State (Rydbergs)	Atomic Radius (Bohr-Units)
Copper		
Hartree-Fock	.54	4.42
Thomas-Fermi	.87	3.13
Silver		
Hartree	.45	4.94
Thomas-Fermi	.44	4.34
Gold		
Hartree	.41	5.96
Thomas-Fermi	.41	4.60
Accepted values[a]		
Copper		2.65
Silver		3.01
Gold		3.01
Calculated by others[b]		
Copper		3.16

[a] F. Seitz, The Modern Theory of Solids, op. cit. p. 6

[b] F. Seitz, The Modern Theory of Solids, op. cit. p. 370

TABLE III

Comparison of Calculations and Accepted Values for the Ionization Energy and Cohesive Energy of Copper, Silver, and Gold.

	Ionization[a] Energy (Rydbergs)	Cohesive[b] Energy (K Cal/mole)
Copper		
Hartree-Fock	.33	24.0
Thomas-Fermi	.45	33.75
Silver		
Hartree	.30	18.6
Thomas-Fermi	.30	13.4
Gold		
Hartree	.35	--
Thomas-Fermi	.28	8.08
Accepted values		
Copper	.558[c]	81.2[d]
Silver	.547[c]	69.0[d]
Gold	.666[c]	82.3[d]
Calculated by others		
Copper		33[e]
Gold		49[f]

[a] The potential represents the calculated ionization energy.

[b] The value of the ionization energy represented by the potential was used in the calculation.

[c] L. H. Ahrens and S. R. Taylor, Spectro Chemical Analysis (Addison-Wesley Publishing Co., Inc., Reading, Mass., 1961).

[d] E. Wigner and F. Seitz, The Qualitative Analysis of the Cohesion in Metals, Advances in Research and Applications of Solid State Physics (Academic Press, New York 1955), Volume 1, p. 108.

[e] F. Seitz, Modern Theory of Solids, op. cit., p. 370.

[f] K. Kambe, Cohesive Energy of Noble Metals, Phys. Rev. 99, No. 2, 419-22 (15 June 1955).

DEVELOPMENT OF A NEW POTENTIAL FOR GOLD

The Model

An inspection of the results of the calculations for the noble metals and the results for sodium indicate two major differences: (1) The sodium potential actually represented the ionization energy, the others did not; and (2) the sodium results agree with experiment, the others did not. If a potential could be found which satisfied the ionization energy, the exchange energy and interaction energies would be taken into account. This statement would not be entirely correct except for a spherically symmetric model, unless the potential itself were a function of angle as well as position. If it were possible to construct a potential which does satisfy the ionization energy, which is spherically symmetric and would give results close to experiment, the simplicity of the original Wigner-Seitz method would be preserved.

Starting the Problem

Fig. 7 shows the Hartree function Z(r) and the Thomas-Fermi potential plotted on the same log-log plot. Z(r) was substituted for $\emptyset(r)$ in the Wigner-Seitz calculation and was found to represent an ionization energy of approximately one Rydberg.

It was decided to try a variation of curves between the limits of the Z(r) Hartree function and the Thomas-Fermi potential to determine which functions satisfied the ionization potential.

It is noted from Fig. 7 that the form of the Z(r) function breaks at r = 3.0. The function then approaches $1/Z$ at approximately r = 6.5. This suggested considering the $\emptyset(r)$ as made up of three curves,

$$0 \leq r \leq 3.0$$
$$3.0 \leq r \leq 6.5$$
$$r \geq 6.5$$

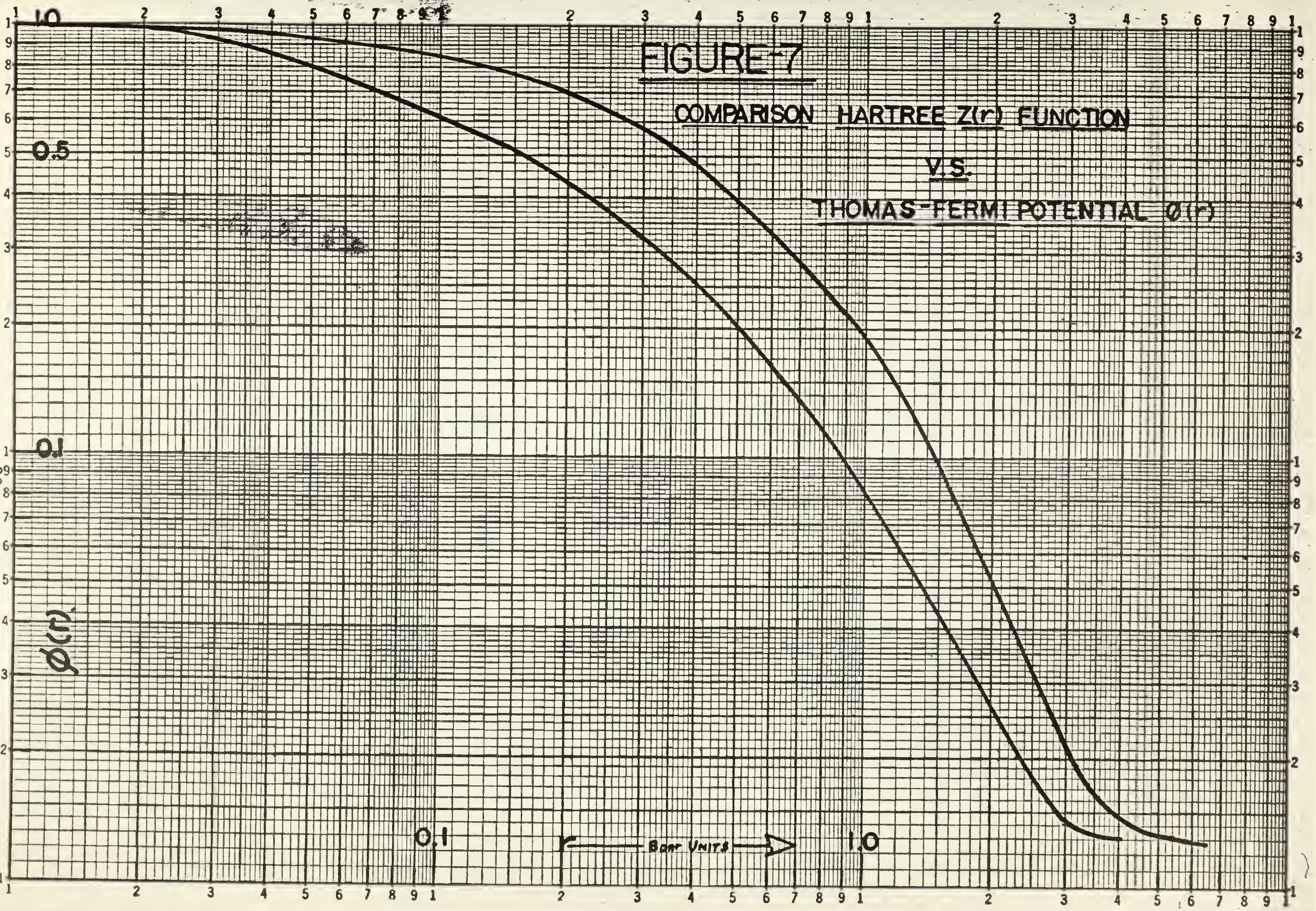

FIGURE-7

COMPARISON HARTREE Z(r) FUNCTION

V.S.

THOMAS-FERMI POTENTIAL Ø(r)

It was necessary to start some place, so it was decided to hold the point r = 3.0, Ø(r) = 0.21 (the values of Z(r) at r = 3.0) and to insure continuity of slope of the two curves joining at r = 3.0.

Development of the Form of the Equations

Since the potential should be periodic between ion cores in the lattice a periodic potential was considered as a starting point. Since Ø(r) is equal to one when r equals zero, a cosine function represents a satisfactory form of a periodic function. (See Fig. 8)

A decay parameter was introduced with the cosine function to develop the shape of the curve that is characteristic of Z(r) and Ø(r)

that is $\phi(r) = e^{-ST\cdot r^{SU}} \mathrm{COS}(SY\cdot r)$

where ST, SY and SU are arbitrary functions.

The periodicity conditions require $\mathrm{COS}(SY\cdot r) = 0$

where $r = \frac{A_0}{4}$

Thus $SY\cdot\frac{A_0}{4} = \frac{\pi}{2}$ OR $SY = \frac{2\pi}{A_0} = .825$

In order that Ø(r) be some finite value other than zero when $r = \frac{A_0}{4}$ the following form was chosen:

$$\phi(r) = (1-SX)\mathrm{EXP}(-ST\cdot r^{SU})\mathrm{COS}(SY\cdot r)+SX$$

Thus Ø(r) is a function of four parameters and has the required form. (See Fig. 9)

In the range $3.0 \leqslant r \leqslant 6.5$, Ø(r) was assumed to vary as $1/r$ with the equation

$$\phi(r) = .021\,\frac{(3+SB)}{(r+SB)} \qquad \text{(See Fig. 10)}$$

using the condition r = 6.5, $\phi(r) = \frac{1}{Z}$

$$\longrightarrow \quad \frac{1}{Z} = .021\,\frac{(3+SB)}{(6.5+SB)}$$

solving the equation for SB yields SB = 2.0

therefore

$$\phi(r) = \frac{.110}{r+2.0} \qquad 3.0 \leqslant r \leqslant 6.5$$

Satisfying the Boundary Conditions

The first condition is: Ø(r) = .021   r = 3.0

$$\longrightarrow .021 = (1-SX)\,EXP(-ST\cdot 3^{SU})\,COS(3\,SY) + SX$$

solving for $\exp(ST\cdot 3^{SU})$

$$EXP(ST\cdot 3^{SU}) = \frac{(1-SX)\,COS(SY\cdot 3)}{(.021-SX)}$$

taking the natural logarithm of both sides

$$ST\cdot 3^{SU} = LN\left(\frac{(1-SX)COS(3\,SY)}{(.021-SX)}\right)$$

taking the natural logarithm of both sides and solving for SU

$$SU = \frac{1}{LN\,3.0}\left\{LN\;LN\left(\frac{(1-SX)COS(3\cdot SY)}{.021-SX}\right) - LN\,ST\right\}$$

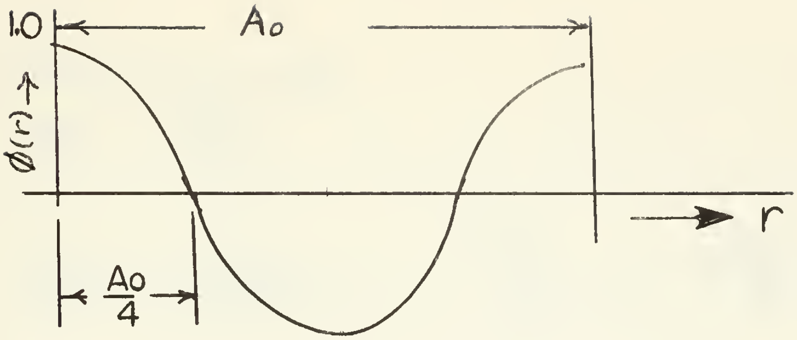

Fig. 8. First Approximation to a Periodic Potential Between Ion Cores. Ao equals the edge length of the fundamental cube of a cubic lattice.

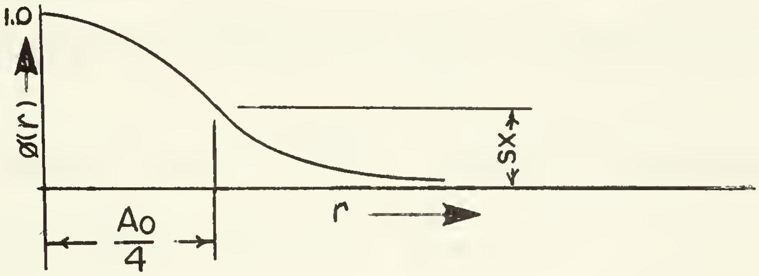

Fig. 9 Graphical Portrayal of the Equation $\varnothing(r) = (1-SX)\mathrm{EXP}(-ST\,r^{SU})\mathrm{Cos}\,SY\cdot r+SX$

SY equals Ao/ 4 , SX is the value of Ø(r) when $SY\cdot r$ equals $\pi/2$

This equation applies in the region $0 \leqslant r \leqslant 3.0$ Bohr Units.

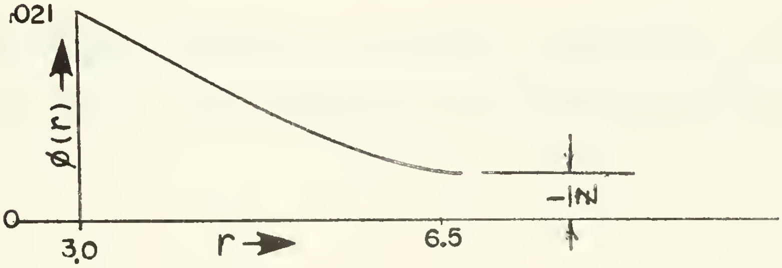

Fig. 10. Graphical Portrayal of the Equation $\varnothing(r) = \frac{.110}{(2.0+r)}$

This equation applies in the range $3.0 \leqslant r \leqslant 6.5$ Bohr Units.

Z is the atomic number.

To satisfy continuity of slope

$$\emptyset(r) = \frac{.110}{r+2}$$

$$\emptyset'(r) = -\frac{.110}{(r+2)^2} = -\frac{\emptyset(r)}{r+2} = -\frac{.021}{5}$$

from the first equation

$$\emptyset'(r) = (1-SX)\cdot EXP(-ST\cdot r^{SU})\left[-SY\cdot SIN(SY\cdot r) - COS(SY\cdot r)\cdot ST\cdot SU\cdot r^{SU-1}\right]$$

This simplifies to

$$\emptyset'(r) = (1-SX)EXP(-ST\, r^{SU})COS(SY\cdot r)\left[-SY\cdot TAN(SY\cdot r) - ST\cdot SU\frac{r^{SU}}{r}\right]$$

since $(1-SX)\ \exp(-ST\cdot r^{SU}) \cdot \cos(SY\cdot r) = \emptyset(r) - SX$

introducing the values of Ø(r) at r = 3.0

$$-\frac{.021}{5} = -(.021-SX)\left(SY\cdot TAN(3\cdot SY) - SU\cdot ST\frac{3^{SU}}{3}\right)$$

Let $ST\cdot 3^{SU} = SZ$

solving for SU

$$SU = \left(\frac{.021}{5(.021-SX)} - SY\cdot TAN(3\cdot SY)\right)\frac{3}{SZ}$$

This value of SU satisfies both boundary conditions. To differentiate between the values of the parameters satisfying one or two boundary conditions

Let SU satisfy one boundary condition and be described by equation

$$SU = \frac{1}{\mathrm{LN}\ 3.0}\left\{ \mathrm{LN}\ \mathrm{LN}\left(\frac{(1-SX)\cdot \mathrm{COS}(3\cdot SY)}{.021-SX}\right) - \mathrm{LN}\ ST \right\}$$

ST is a parameter in the equation satisfying one boundary condition.

$$SU1 = \frac{3}{SZ}\left(\frac{.021}{5(.021-SX)} - SY\cdot \mathrm{TAN}(3\ SY)\right)$$

$$SZ = SA\cdot 3^{SU1}$$

SZ is a parameter used in the equation satisfying two boundary conditions.

The reason for the above step is not obvious but will become clear in the next section.

The relationship between SA , LN SX , and SY is portrayed in Fig. 11. Each point meets the two boundary conditions (1) holding the point 0(r) = .021 at r = 3.0, (2) continuity of slope at r = 3.0.

If one one boundary condition is held constant 0(r) = .021 at r = 3.0 (Fig. 12) and a fixed value of SX and SY are substituted in the cellular calculation for E = .666 Rydbergs, then ST is varied until a value of ST brackets the ionization energy. That is, in Fig. 13 the value of R(r) changes from minus to plus.

In this manner the SY curves are developed by varying SX.

When the two curves are superimposed the intersection meets all the boundary conditions (Fig.14). This procedure proved necessary as the slope of SX/SA was very flat and made location of the point of intersection difficult when all the conditions were wrapped into one equation. In this method there are two curves intersecting at right angles and it is easier

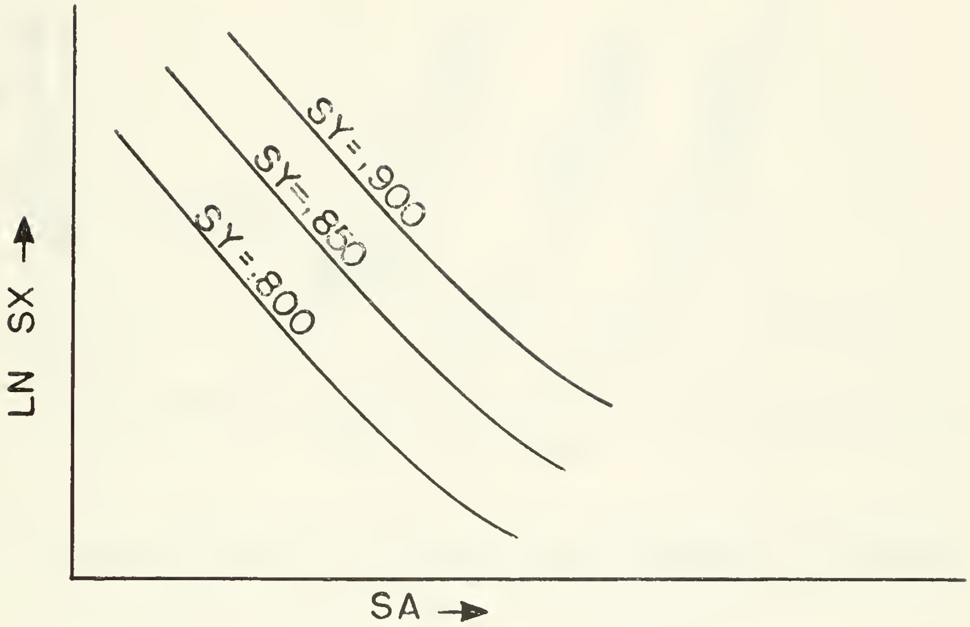

Fig. 11. The First Step in the Variational Procedure. A Semi-Log Plot of Curves of Constant SY vs. SX and SA.

Points on the SY curve satisfy the boundary conditions

$\phi(r) = .021$ at $r = 3.0$ and continuity of slope at $r = 3.0$.

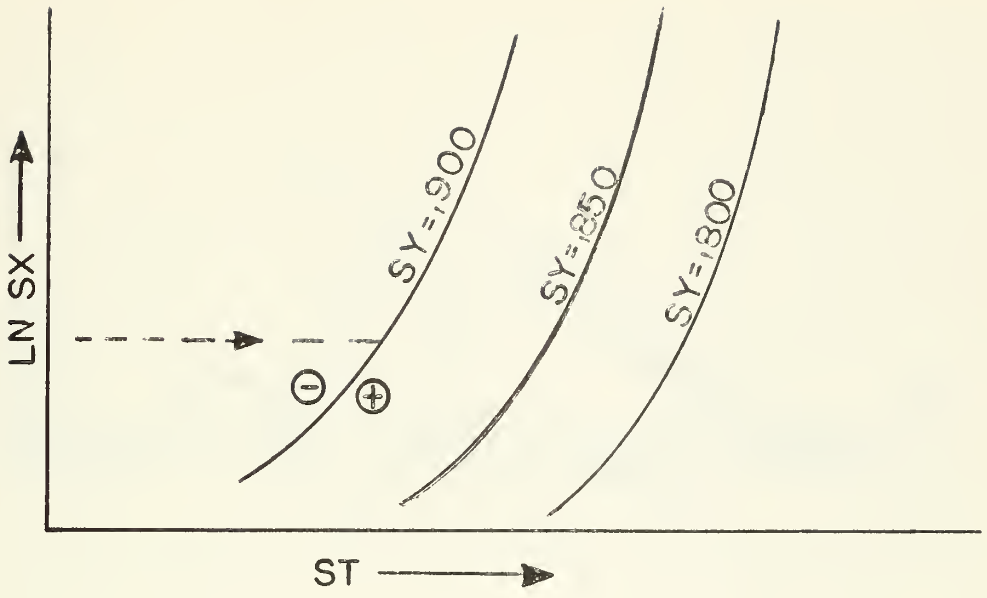

Fig. 12. The Second Step in the Variational Procedure. A Semi-Log Plot of Curves of Constant SY vs. ln SX and ST.

Points on the SY curves satisfy the boundary conditions: the ionization = .666 Rydbergs and Ø(r) = 0.21 at r = 3.0. Initially SX and SY are held constant and ST is varied. The triad SY, ST and SX determine Ø(r). The radial wave function R(r) is determined by Ø(r). When R(r) changes sign at r = 8.2 Bohr units the ionization energy is satisfied. Keeping SY constant and using incremental values of SX, the procedure is repeated, giving the curves SY = constant.

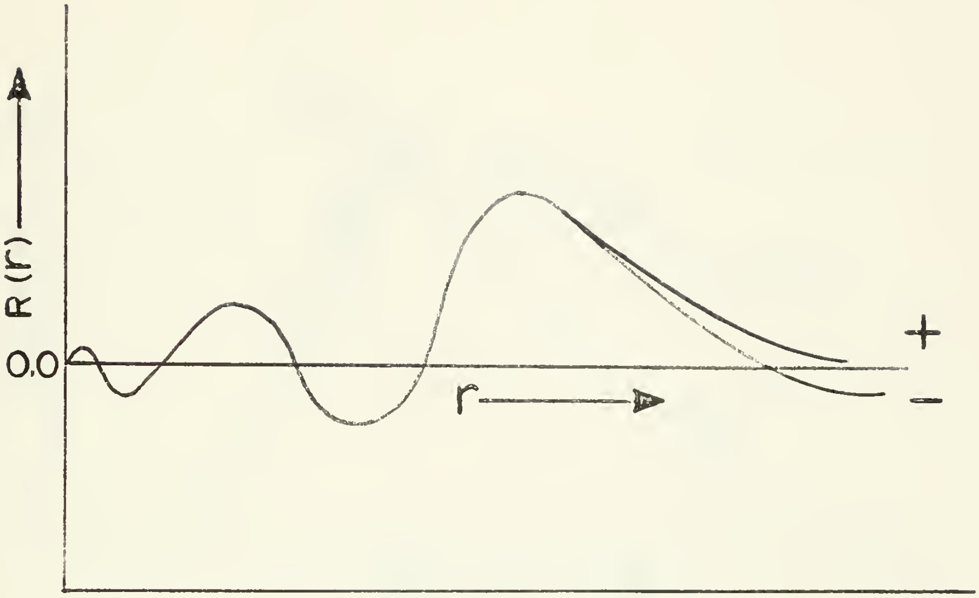

Fig. 13. Determination of the Ionization Energy.

The wave function R(r) which satisfies the ionization energy lies between the limits of the curves marked + and -.

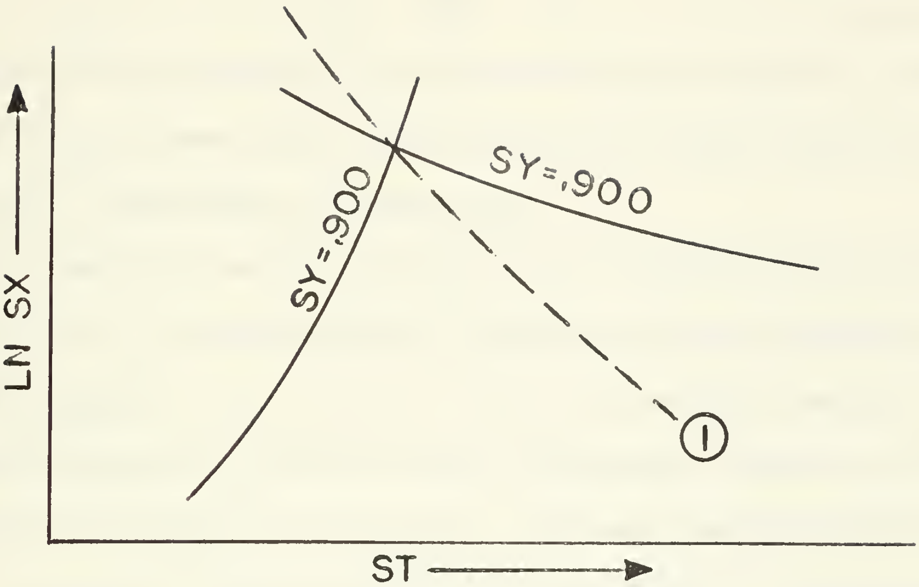

Fig. 14. Step Three of the Variation Procedure.

This plot is a superposition of Figs. 11 and 12. The point of intersection of curves of constant SY satisfy the boundary conditions Ø(r) = 0.21 at r = 3.0, continuity of slope at r = 3.0 and the ionization energy = .666 Rydbergs. The curve marked ① represents the locus of points satisfying the boundary conditions for various values of SY.

to select the intersection.

The results of the variation indicated that the boundary conditions were met along the curve marked ① in Fig. 14. This was surprising. An additional criterion was then invoked that was to pick the curve which gave either the lowest energy state or values of atomic radius and cohesive energy that corresponded to known values.

The results of the first variation are tabulated in Table IV. (See also Fig. 15.) A second series of variations was made perturbing the boundary condition $r = 3.0$, $\phi(r) = .021$. This boundary condition was originally selected as starting point by observing a break in the shape in the Hartree $Z(r)$ curve at this point. The entire procedure depicted in Figs. 11 through 15 was repeated for new dyad $\phi(r)$, r, representing a new boundary condition. The second variation was terminated when the accepted value of the atomic radius was obtained. The results of the second variation are tabulated in Table IV. It is noted that the cohesive energy from the derived potential, 81.6 Rydbergs, compares very well with the accepted value 83.5 Rydbergs.

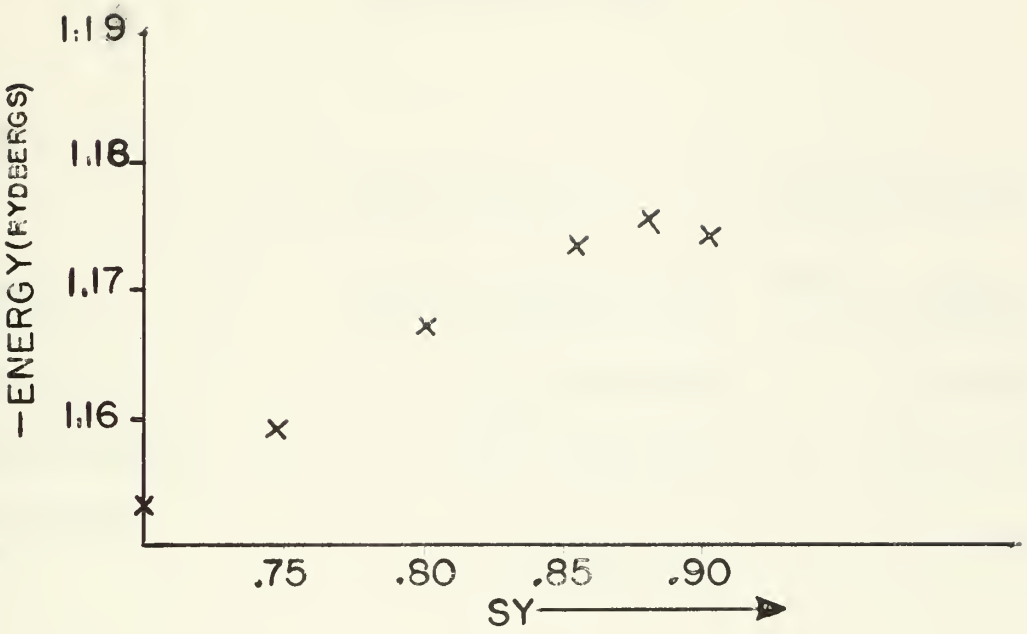

Fig. 15. Plot of Values of the Lowest Energy State vs. SY Satisfying the Boundary Condition, the Ionization Energy = .666 Rydbergs. The values of SY giving the lowest value of the energy state represents the triad of parameters from curve ① in Fig. 14. This triad determines $\emptyset(r)$.

TABLE IV

RESULTS OF THE FIRST AND SECOND VARIATIONS FOR GOLD

	First Variation	Second Variation
Boundary Condition	$\phi(r) = .021$ $r = 3.0$ Bohr units	$\phi(r) = .020$ $r = 2.99$ Bohr units
Atomic Radius[a]	3.13 Bohr units	3.01 Bohr units
Cohesive Energy[b]	80.6 K Cal/Mole	81.6 K Cal/Mole
Lowest Energy State	1.172 Rydbergs	1.194 Rydbergs

Note: [a] Accepted Value of r_o = 3.01 Bohr units.

[b] Accepted Value of Cohesive Energy = 83.5 K Cal/Mole

CONCLUSIONS AND SUMMARY OF RESULTS

It proved possible to construct a potential for gold which can be expressed in a closed form and when used in the cellular method can furnish very close agreement with accepted values of the atomic radius and the cohesive energy. This potential is a central field potential and represents a spherically symmetric model. The potential $V(r)$ is expressed in terms of a function, $\text{Ø}(r)$, which is the normalized contribution to the effective potential.

$$\text{Ø}(r) = .9174\ \mathrm{EXP}(-1.429\, r^{.524676})\, \mathrm{COS}(.875\, r) + .0826$$

$$0 \leq r \leq 2.99 \qquad \text{Bohr units}$$

$$\text{Ø}(r) = \frac{.121}{3.062 + r}$$

$$2.99 \leq r \leq 6.5 \qquad \text{Bohr units}$$

$$\text{Ø}(r) = \frac{1}{79}$$

$$r \geq 6.5 \qquad \text{Bohr units}$$

Fig. 16 graphically portrays the complete Wigner-Seitz Cellular Computation for gold using the potential as described above.

It is very difficult to find any work on gold with which to compare our results. Kambe[22] made a calculation of the cohesive energy of gold

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[22] K. Kambe, Phys. Rev. 99, No. 2, 419-22 (July 15, 1955)

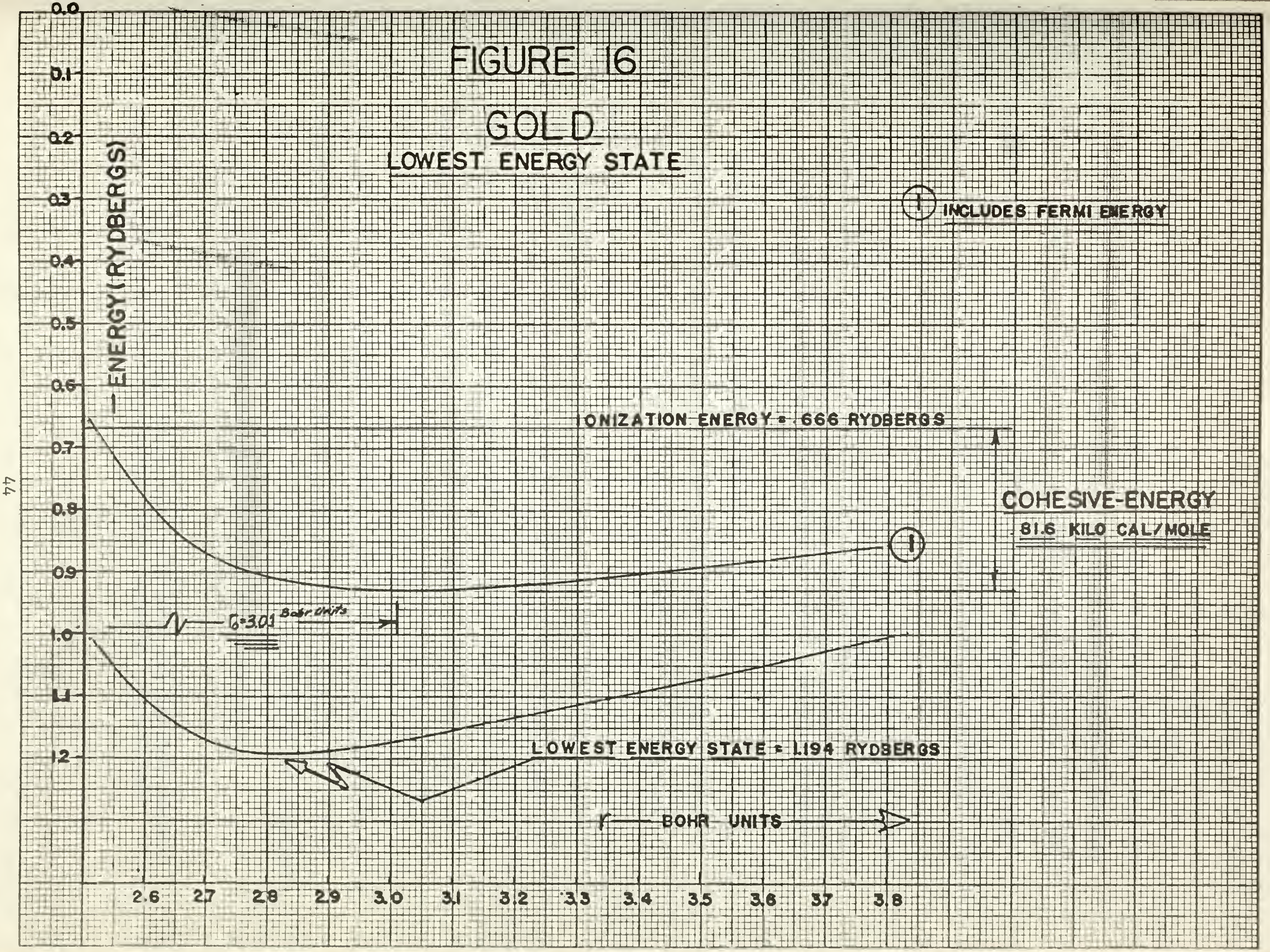

FIGURE 16

GOLD

LOWEST ENERGY STATE

and obtained a value of 49 kilo calories per mole. Segall[23] made a calculation of the energy bands in gold at lattice symmetry points using the Hartree Potential. His results indicate a lowest energy state of approximately 1.25 Rydbergs in the (0,0,0) and $\frac{2\pi}{a}(1/2,1/2,1/2)$ direction, and approximately 1.3 Rydbergs in the $\frac{2\pi}{a}(1,0,0)$ direction. The following quote is made from Segall[23] to indicate his opinion on the uncertainty of the potential for gold.

> The difficulties already discussed for Ag, in obtaining a good potential, are more severe for Au because it is a considerably heavier atom. Also, at present, only Hartree functions are available. Thus we would expect considerably more uncertainty in the potential which we have constructed in the same manner as for Cu and Ag, and consequently in the final results.

Contribution to the Cohesive Energy

There is a marked difference between the cohesive energy calculated using the Hartree and Thomas-Fermi Potential (Table III) and the newly developed potential.

An examination of the wave function R(r) of the state corresponding to the ionization energy for the free ion potential for the Hartree (Fig. 70) or the Thomas-Fermi Potential (Fig. 63) indicates a 6S wave function. If these are compared with the radial wave function R(r) of the calculated potential (Fig. 17), or $\psi(r)$ (Fig. 18) or $\psi(r)\cdot\psi^*(r)$ (Fig. 19), there is a marked difference. The first difference is the new potential indicates a 7S instead of a 6S state. Secondly, the inner shells appear more tightly bound. One interpretation based on the examination of the functions discussed above would be that there is a

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[23] B. Segall, Theoretical Energy Band Structures for the Noble Metals (General Electric Research Laboratory, 1961) Report Nr. 61 R1(2785G)

FIGURE 17
GOLD
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
ENERGY STATE E = .666 RYDBERGS
IONIZATION ENERGY

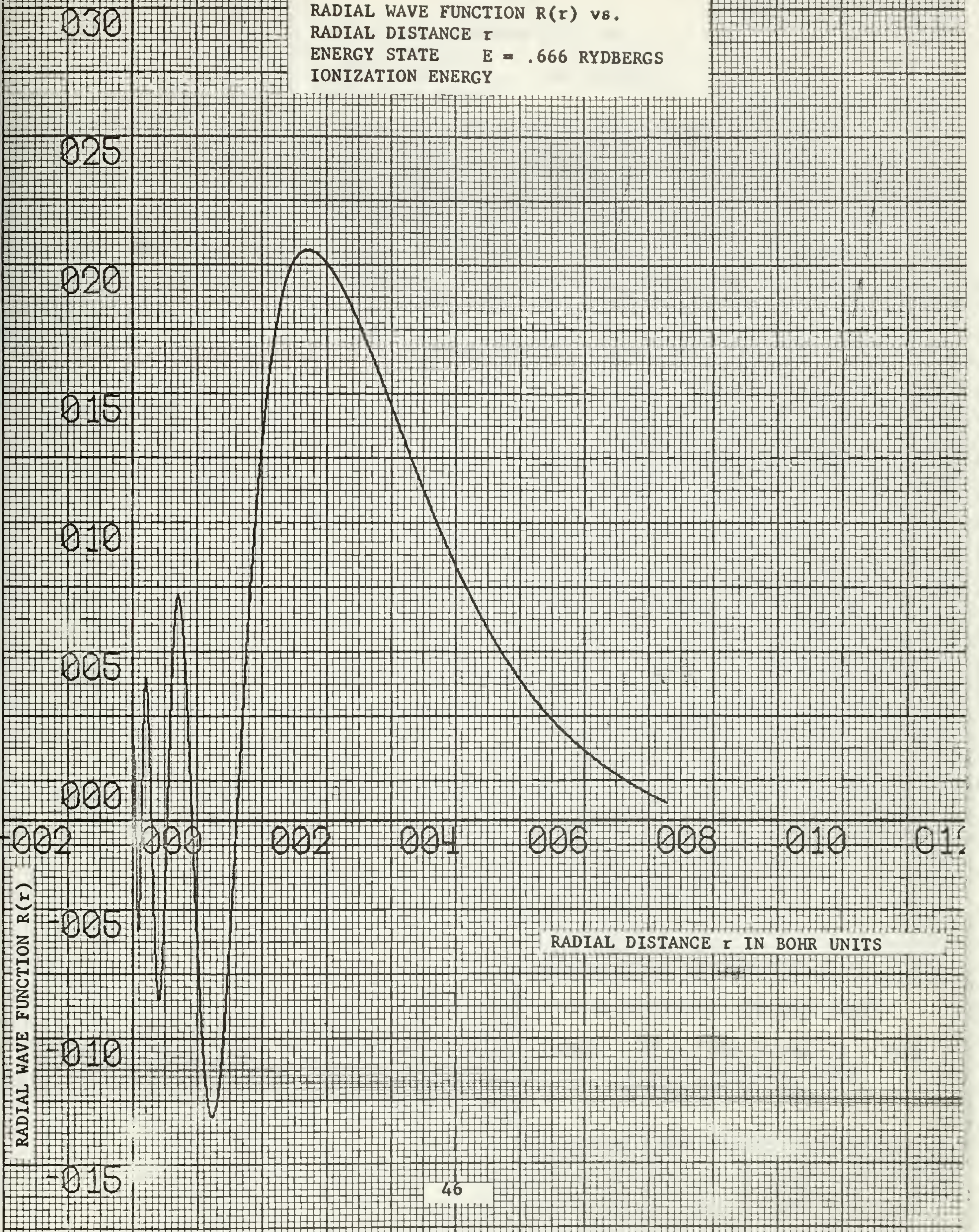
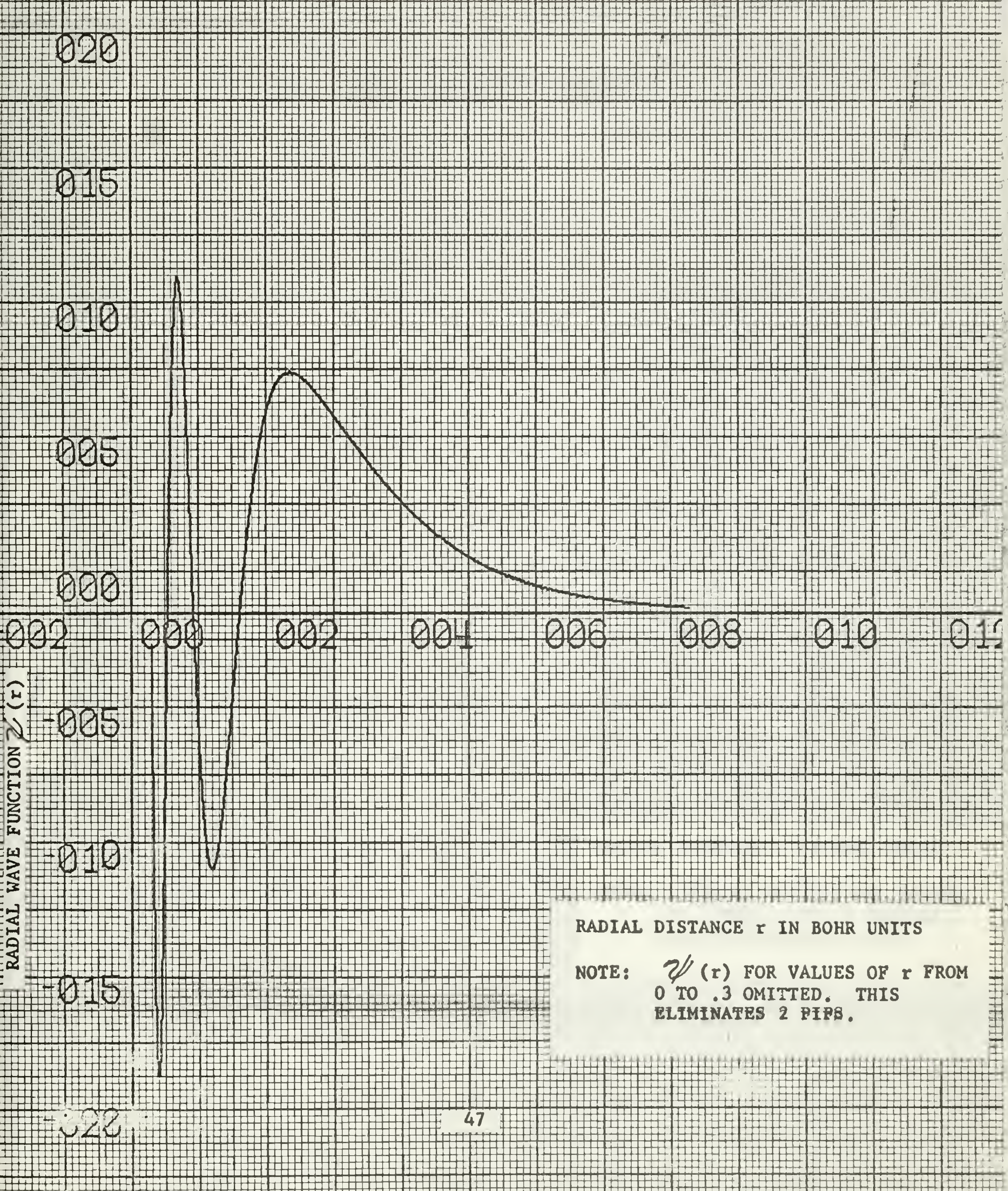


FIGURE 18
GOLD
RADIAL WAVE FUNCTION $\psi(r)$ vs.
RADIAL DISTANCE r
ENERGY STATE E = .666 RYDBERGS
IONIZATION ENERGY



RADIAL DISTANCE r IN BOHR UNITS

NOTE: $\psi(r)$ FOR VALUES OF r FROM 0 TO .3 OMITTED. THIS ELIMINATES 2 PIPS.

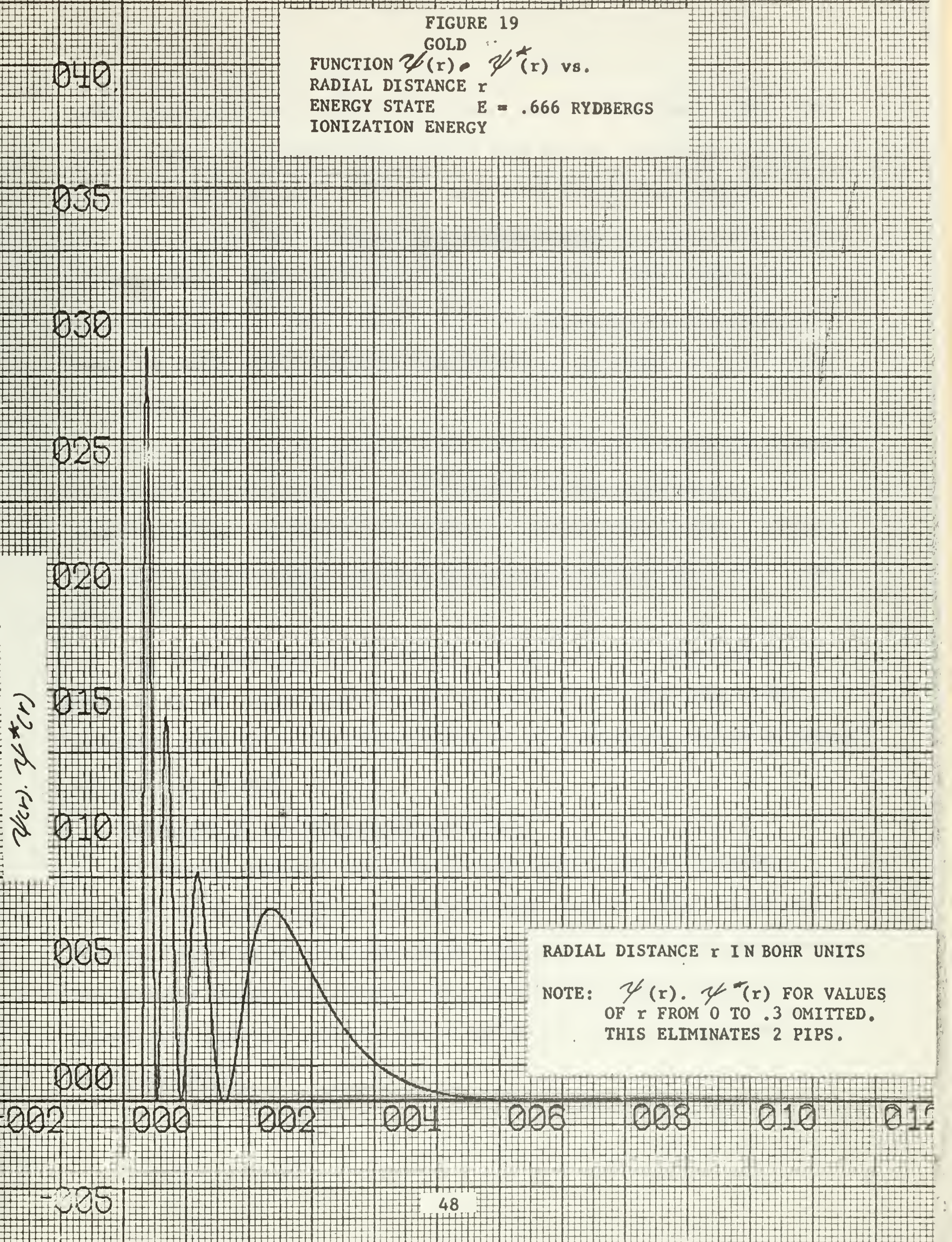


FIGURE 19
GOLD
FUNCTION $\psi(r) \cdot \psi^*(r)$ vs.
RADIAL DISTANCE r
ENERGY STATE E = .666 RYDBERGS
IONIZATION ENERGY

RADIAL DISTANCE r IN BOHR UNITS

NOTE: $\psi(r) \cdot \psi^*(r)$ FOR VALUES OF r FROM 0 TO .3 OMITTED. THIS ELIMINATES 2 PIPS.

redistribution of the electrons in a metal when compared with a free ion. The 6S appears to be more tightly bound than the 5f. There is a strong indication that there is a material overlap of these outer orbitals. It thus appears that the difference in cohesive energy is accounted for by a strong exchange interaction between the 5f orbitals. The difference between the two calculated values, 8.08 K Cal/Mole for the Thomas-Fermi potential and 81.6 K Cal/Mole for the developed potential, is substantial and striking.

The validity of the physical interpretation must of course be tempered by the assumptions that went into the model for the calculations. It appears that the calculation in this paper indicates the limit of a Wigner-Seitz cellular calculation using a spherically symmetric model for a heavy metal.

The wave functions for the lowest energy state are indicated in Figs. 20 to 22. It is noted that $\psi(r)$ is practically flat over a considerable range of r. The wave functions for intermediate values of energy are depicted in Figs. 23 to 26.

Extension of the Variational Technique

It appears possible, using the present calculations to develop a potential which when used in the Schroedinger equation would satisfy the boundary condition on the Wigner-Seitz polyhedron. It may be surmised that the cohesive energy calculated in this manner would differ from the spherically symmetric model by only 1.5% (83.5 K Cal/Mole, compared to 81.6 K Cal/Mole).

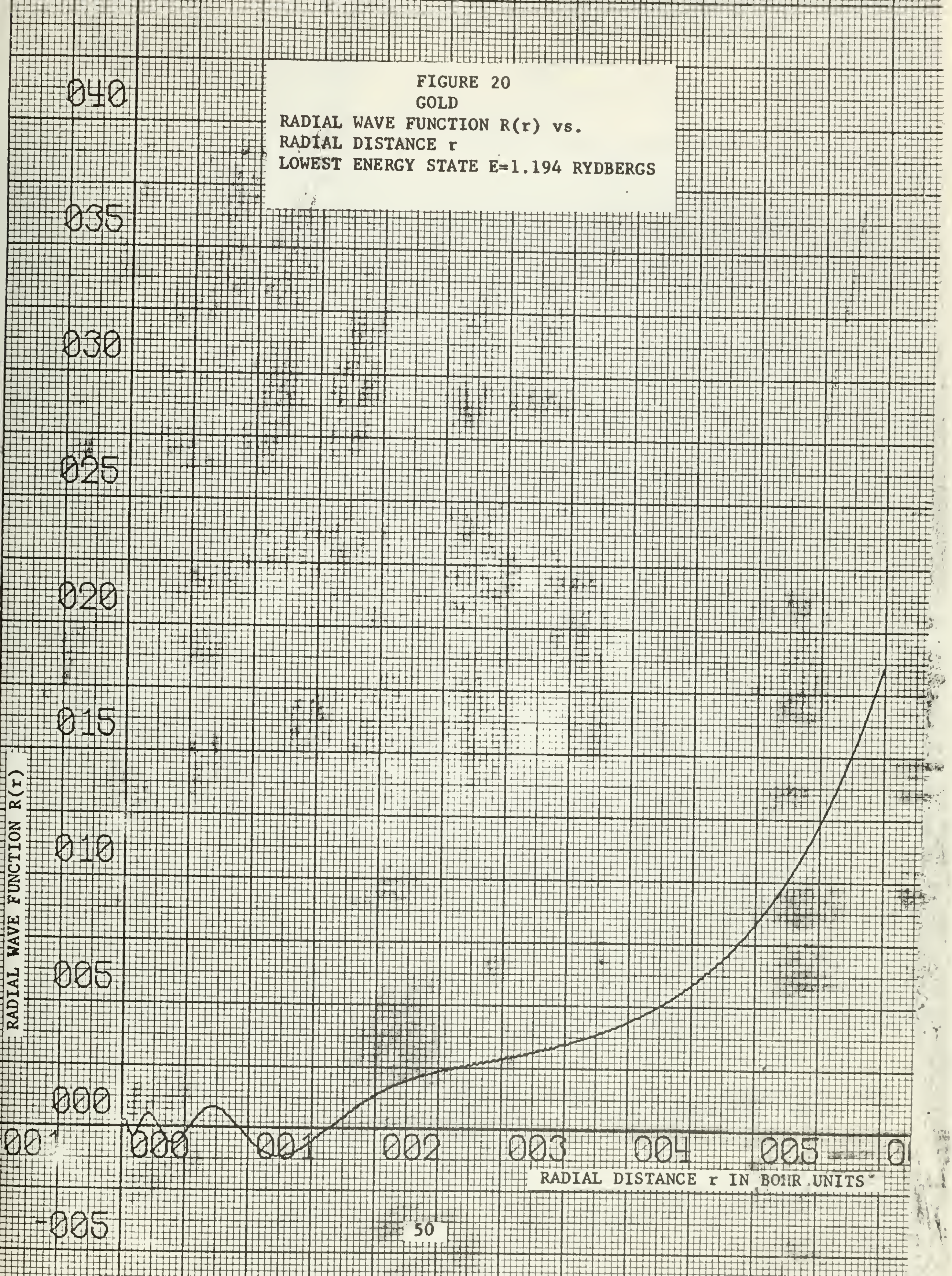


FIGURE 20
GOLD
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
LOWEST ENERGY STATE E=1.194 RYDBERGS

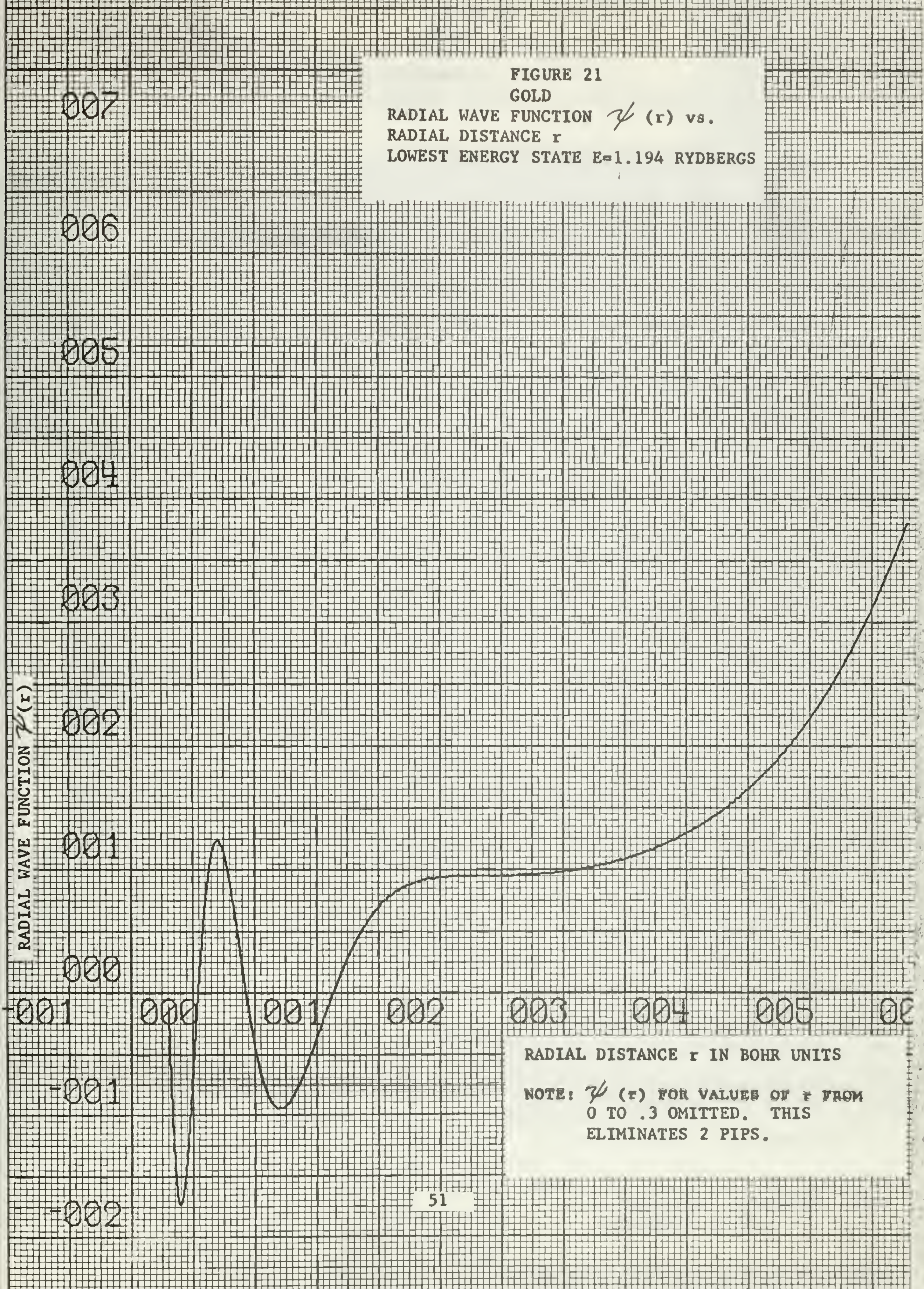
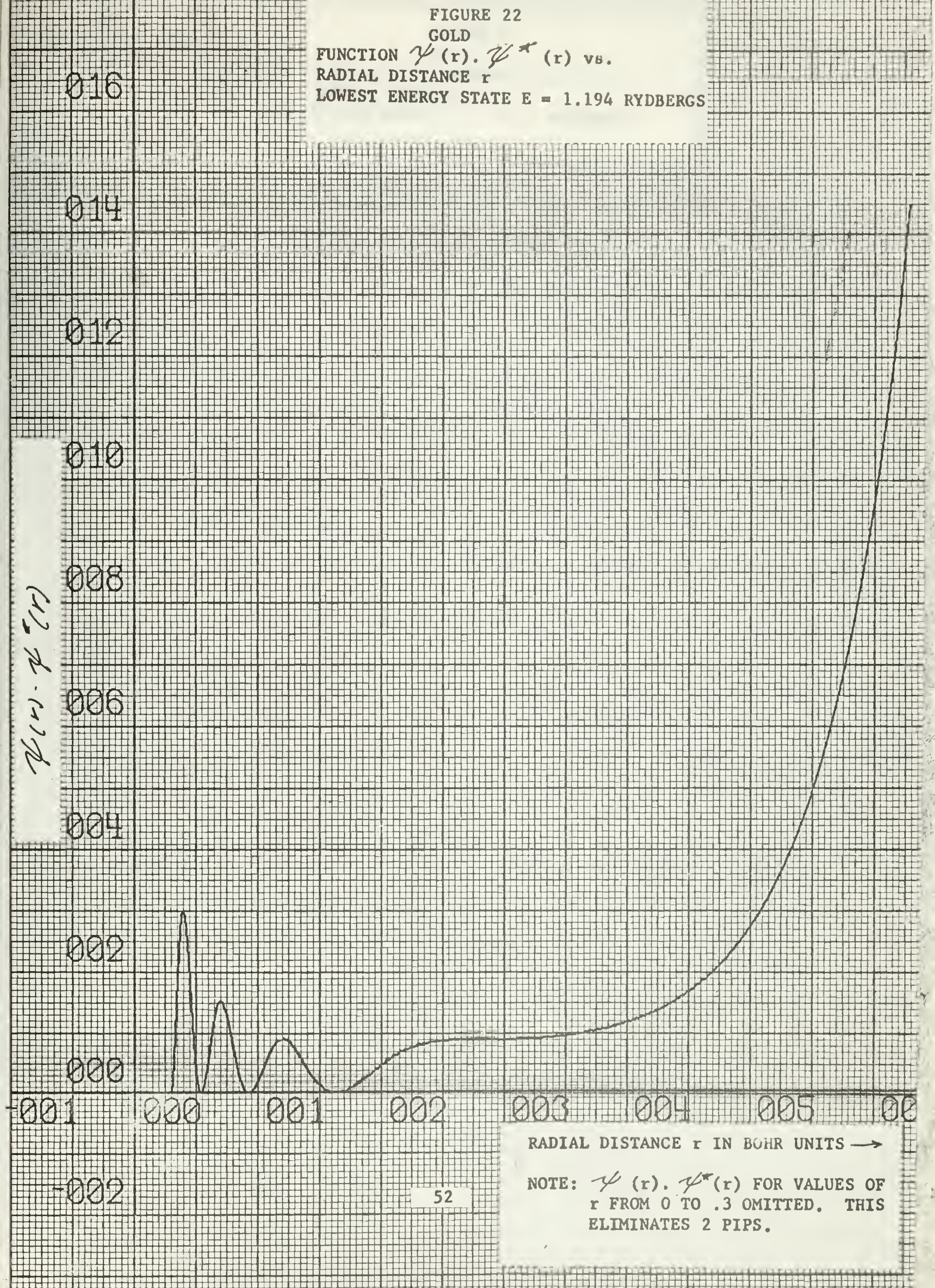


FIGURE 21
GOLD
RADIAL WAVE FUNCTION ψ (r) vs.
RADIAL DISTANCE r
LOWEST ENERGY STATE E=1.194 RYDBERGS

RADIAL DISTANCE r IN BOHR UNITS

NOTE: ψ (r) FOR VALUES OF r FROM 0 TO .3 OMITTED. THIS ELIMINATES 2 PIPS.

FIGURE 22
GOLD
FUNCTION $\psi(r) . \psi^{*}(r)$ vs.
RADIAL DISTANCE r
LOWEST ENERGY STATE E = 1.194 RYDBERGS



NOTE: $\psi(r) . \psi^{*}(r)$ FOR VALUES OF r FROM 0 TO .3 OMITTED. THIS ELIMINATES 2 PIPS.

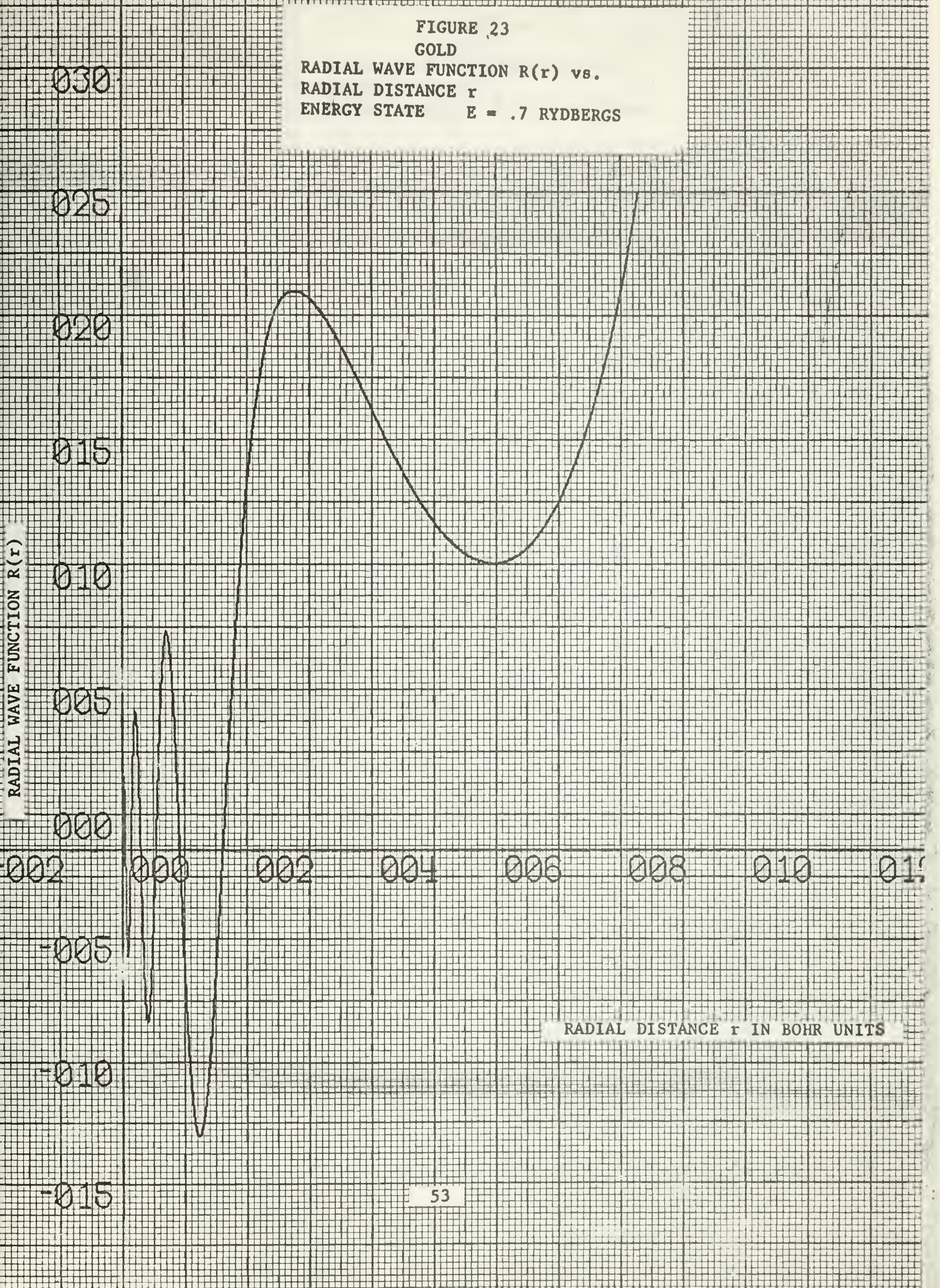
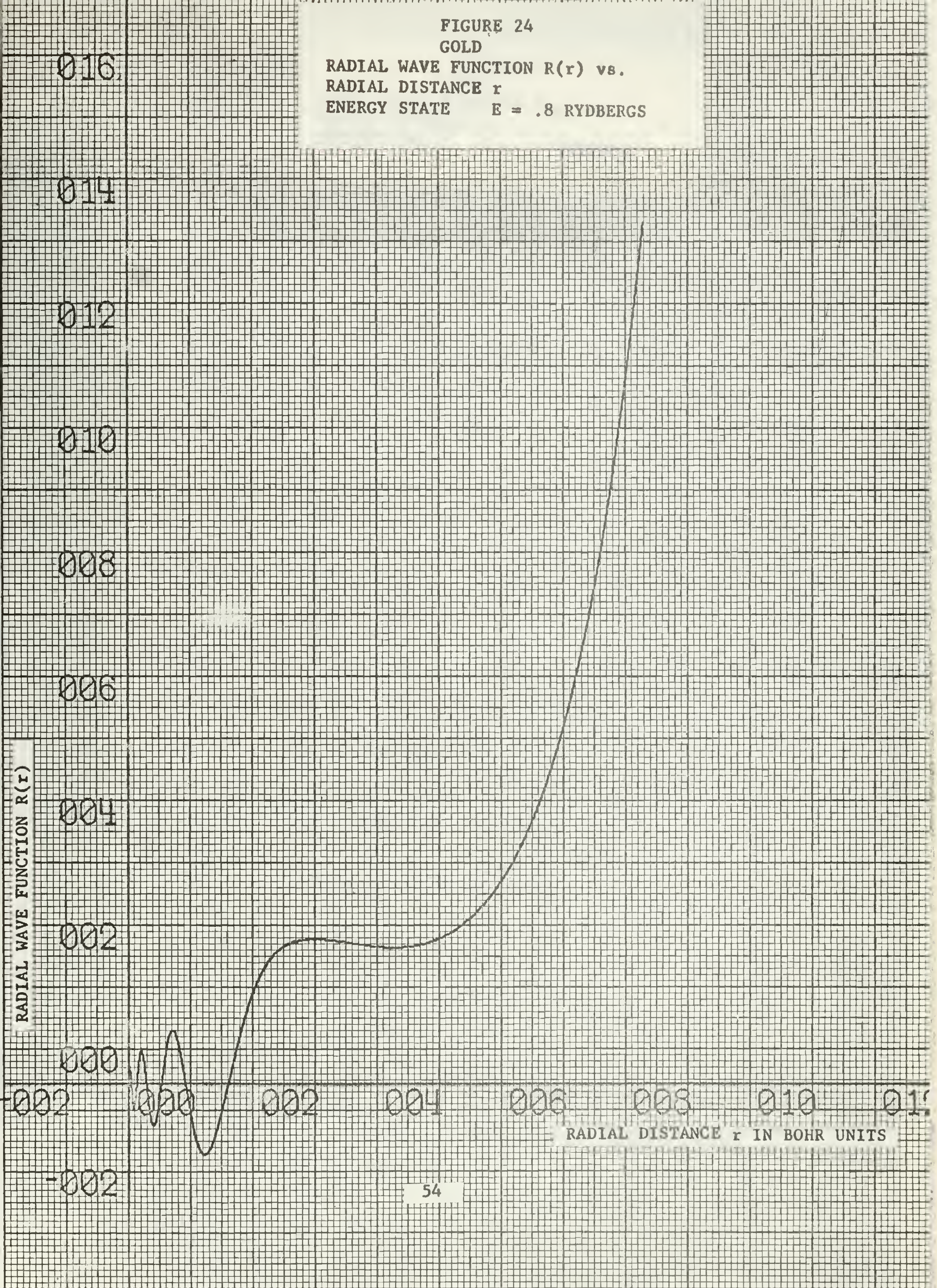


FIGURE 23
GOLD
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
ENERGY STATE E = .7 RYDBERGS

FIGURE 24
GOLD
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
ENERGY STATE E = .8 RYDBERGS



[illegible]

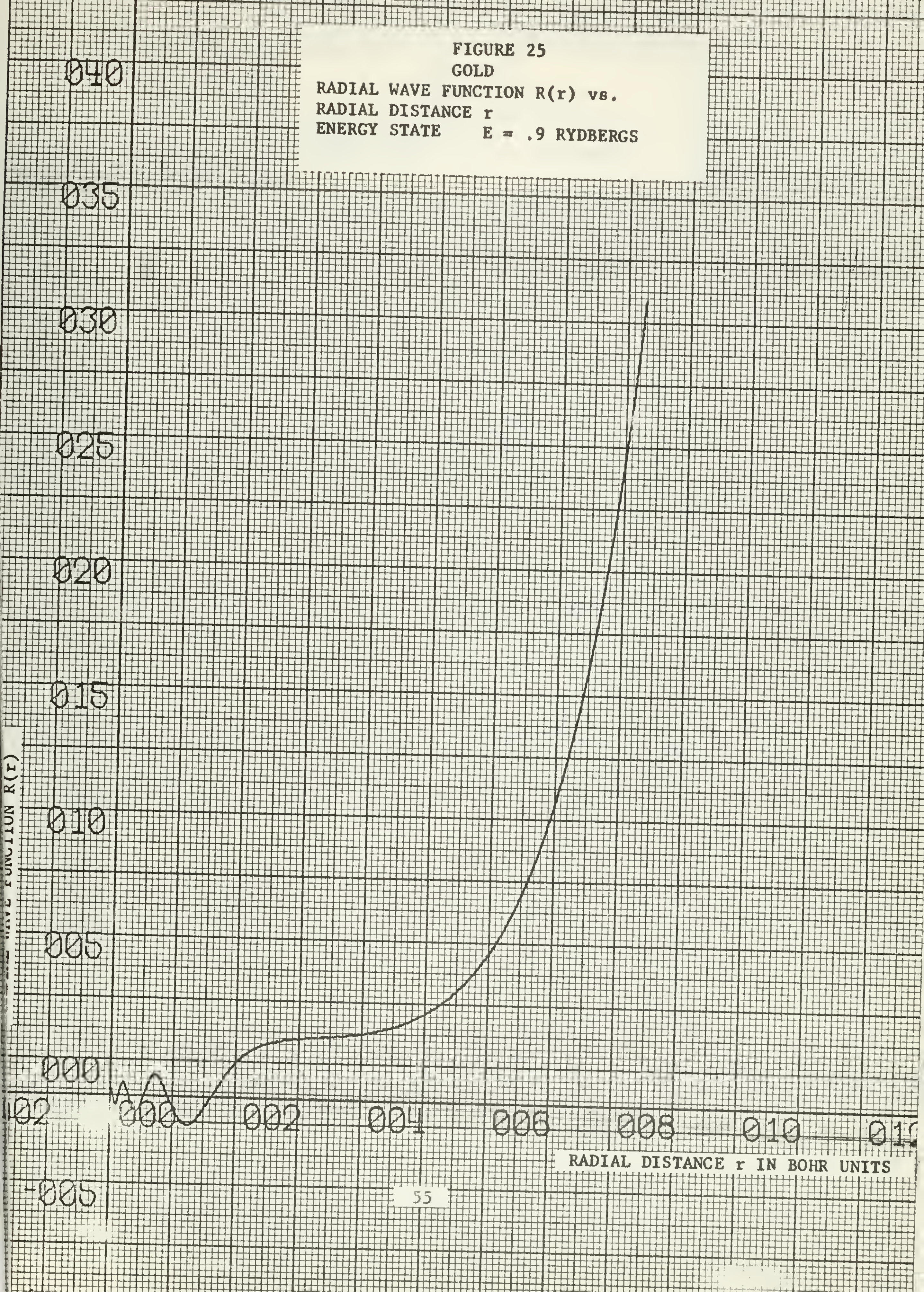


FIGURE 25
GOLD
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
ENERGY STATE E = .9 RYDBERGS

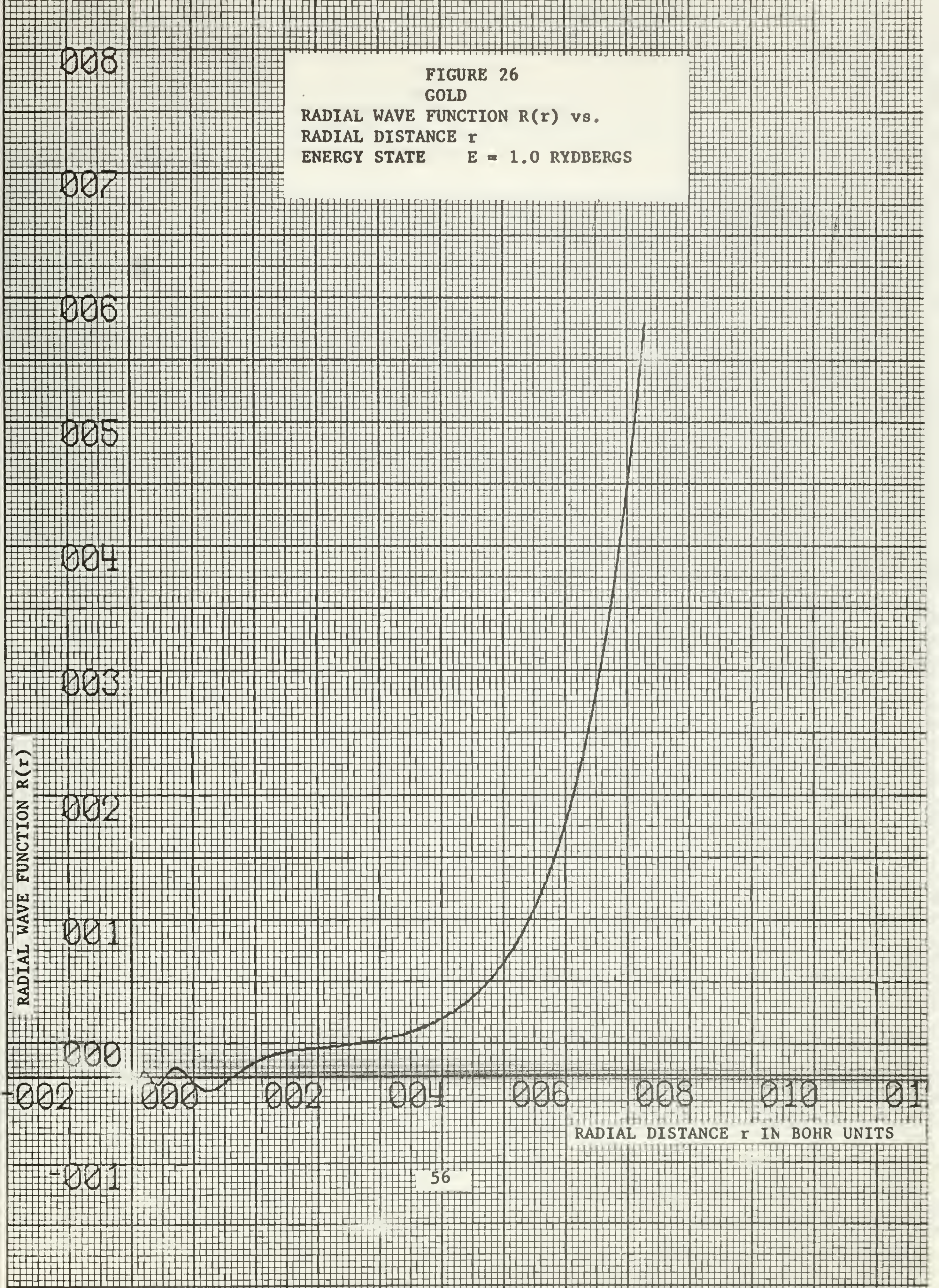


FIGURE 26
GOLD
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
ENERGY STATE E = 1.0 RYDBERGS

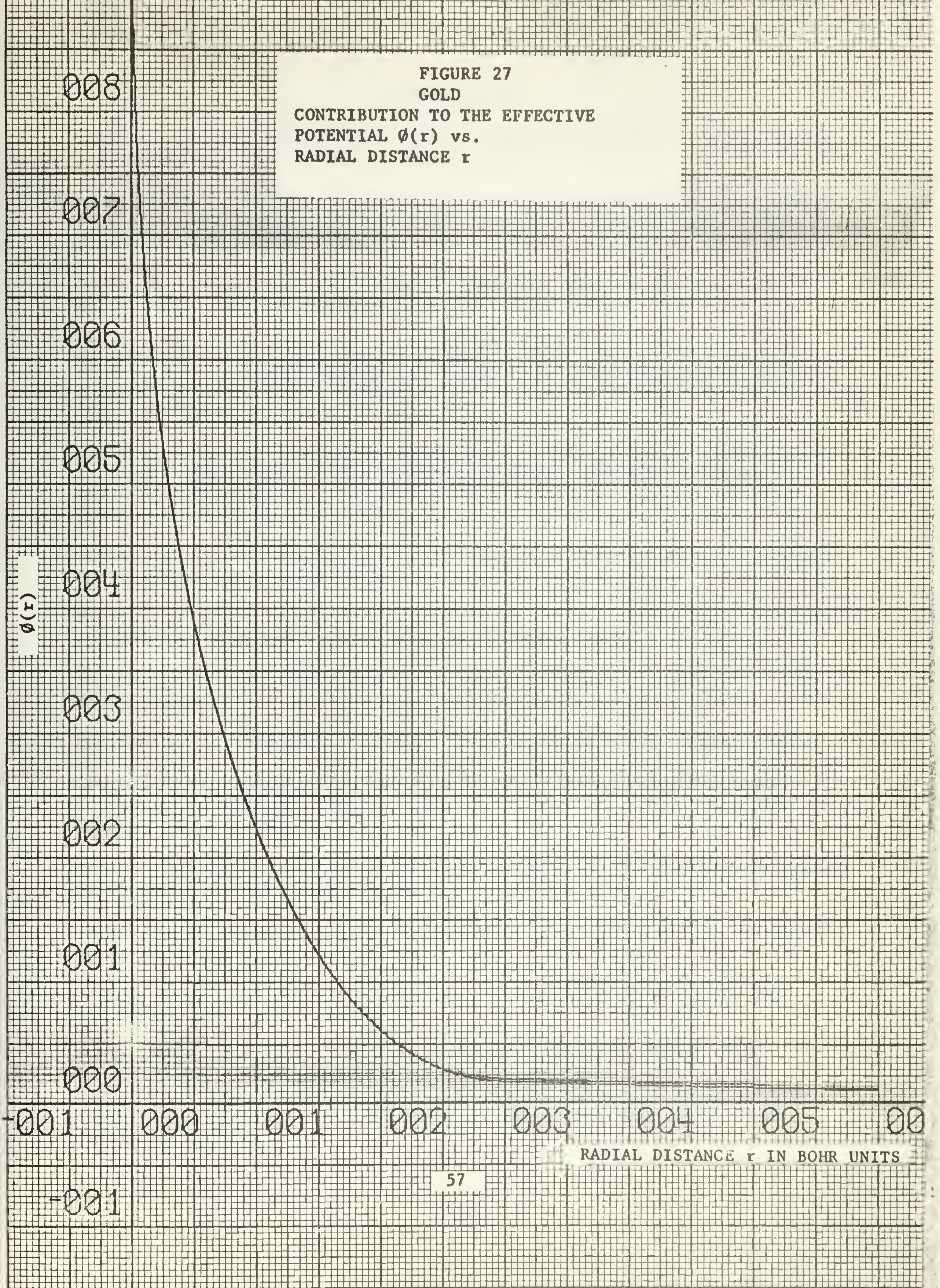


FIGURE 27
GOLD
CONTRIBUTION TO THE EFFECTIVE
POTENTIAL $\phi(r)$ vs.
RADIAL DISTANCE r

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APPENDIX I

DEVELOPMENT OF A SERIES SOLUTION TO THE TRINOMIAL EQUATION

Basic Approach

The equation to be solved is in the form

$$\frac{d^2R}{dr^2} + 2(V(r)-E)R = 0 \qquad [I-1]$$

with $V(r) = \frac{Z\,\emptyset(r)}{r}$

Z = atomic number

Ø(r) = known function of r

r = radius in units of Bohr radii

E = energy in units of 2x Rydbergs = 27 e.v

Ø(r) decreases monotomically from

$\emptyset(0) = 1.00$ and approaches $1/Z$ as $r \to \infty$

Since Ø(r) is given, the equation of a parabola through the points 0, 1, and 2 can be determined (Fig. 28a). The equation will be of the form $B + Qr + Tr^2$

Assume Ø(r) is substituted into equation [I-1] and equation [I-1] is solved with suitable initial conditions. Then a solution is available in the range $0 \leq r \leq 2$ (Fig. 28b).

Calculate the values of $R(r)$ AT $r = 1$

$\frac{dR(r)}{dr}$ AT $r = 1$

Now pass a parabola through the points 1, 2 and 3, obtaining an approximation for the function Ø(r) in this range. Then substitute the parabolic approximation into equation [I-1] using as initial conditions the previously calculated values of R(r) and $\frac{dR(r)}{dr}$ at r = 1. The

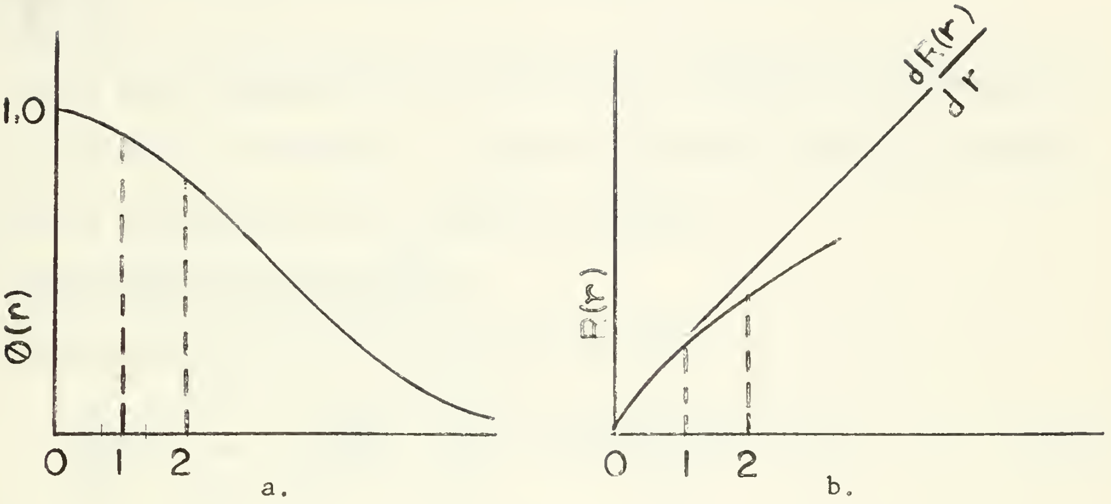


Fig. 28. The Boundary Value Approach.

solution now applies in range $1 < r < 5$. The values of R(r) and $\frac{dR(r)}{dr}$ can now be calculated at midrange.

This process may now be continued as a series of boundary value problems until a complete solution is obtained. If the solution IS CONVERGENT IN EACH INTERVAL THE OVERALL SOLUTION IS CONVERGENT.

A very good approximation to the curve is obtained by evaluating at the half interval. Continuity of slope and position of R(r) is assured since these values are used as initial conditions.

The Solution of the Equation

The equation [I-1] may be put into the form

$$\frac{d^2R(r)}{dr^2} + \left(\frac{BB}{r} + QQ + RR\cdot r\right) R(r) = 0 \qquad \text{[I-2]}$$

where

$$\emptyset(r) = B + Qr + Tr^2$$
$$BB = 2ZB$$
$$QQ = 2ZQ - 2E$$
$$RR = 2ZT \cdot$$

Let $r = e^{\Theta}$ and multiply [I-2] by r^2

$$\left(\frac{r^2d^2}{dr^2} + BB\ r + QQ r^2 + RR\ r^3\right) R(r) = 0 \qquad \text{[I-3]}$$

$\frac{r^2d^2}{dr^2}$ may be represented operationally as $D(D-1)$

$$\frac{r^2d^2}{dr^2} = D(D-1)$$

The solution of the equation $D(D-1)R(r) = 0$ is $R(r) = C_2e^{\Theta} + C_1$

[24] G. Boole, op, cit.

Thus [I-3] may be written

$$\left(D(D-1)+BBe^{\theta}+QQe^{2\theta}+RRe^{3\theta}\right)R(r)=0$$

Operating on the left by $\dfrac{1}{D(D-1)}$

$$\left(1+\phi_1(D)e^{\theta}+\phi_2(D)e^{2\theta}+\phi_3(D)e^{3\theta}\right)R(r)=C_1+C_2e^{\theta} \quad \text{[I-4]}$$

where
$$\phi_1(D)=\frac{BB}{D(D-1)}$$
$$\phi_2(D)=\frac{QQ}{D(D-1)}$$
$$\phi_3(D)=\frac{RR}{D(D-1)}$$

Operating on the left by

$$\left(1+\phi_1(D)e^{\theta}+\phi_2(D)e^{2\theta}+\phi_3(D)e^{3\theta}\right)^{-1}=\Phi(D)^{-1}$$

$$R(r)=\Phi^{-1}(D)\left\{C_1+C_2e^{\theta}\right\}$$

$\Phi^{-1}(D)$ may be expanded in the form

$$\sum_i F_i(D)e^{i\theta}=F_0(D)+F_1(D)e^{\theta}+F_2(D)e^{2\theta}+\cdots+F_n(D)e^{n\theta}$$

then $\left(1+\phi_1(D)e^{\theta}+\phi_2(D)e^{2\theta}+\phi_3(D)e^{3\theta}\right)\sum_i F_i(D)e^{i\theta}=1$

The $F_i(D)$ may be evaluated in terms of $\phi_i(D)$ by equating like powers of $e^{n\theta}$ or $e^{i\theta}$

The relation

$$\phi_i(D)e^{n\theta}F_j(D)e^{m\theta} = \phi_i(D)F_j(D-n)e^{(n+m)\theta}$$

is required for the reduction.

Equating coefficients

$$\begin{aligned}
&F_0(D) = 1\\
&F_1(D) = -\phi_1(D)\\
&F_2(D) = -\phi_1(D)F_1(D-1) - \phi_2(D)\\
&F_3(D) = -\phi_1(D)F_2(D-1) - \phi_2(D)F_1(D-2) - \phi_3(D)\\
&F_4(D) = -\phi_1(D)F_3(D-1) - \phi_2(D)F_2(D-2) - \phi_3(D)F_1(D-3)\\
&\vdots\\
&F_n(D) = -\phi_1(D)F_{n-1}(D-1) - \phi_2(D)F_{n-2}(D-2) - \phi_3(D)F_{n-3}(D-3)
\end{aligned}$$

The solution, once the F's are evaluated becomes

$$\begin{aligned}
R(r) &= F_0(D) + F_1(D)e^{\theta} + F_2(D)e^{2\theta} + \dots + F_n(D)e^{n\theta}(C_1 + C_2e^{\theta})\\
&= C_1(1 + F_1(D)e^{\theta} + F_2(D)e^{2\theta} + \dots + F_n(D)\cdot e^{n\theta})\\
&\quad + C_2(e^{\theta} + F_1(D)e^{2\theta} + F_2(D)e^{3\theta} + \dots + F_n(D)e^{(n+1)\theta})
\end{aligned}$$

[I-5]

The Starting Case

In this case the initial conditions are:

$$R(r) = 0 \qquad r = 0 \qquad [I-6]$$

$$\frac{dR(r)}{dr} = 1 \qquad r = 0 \qquad [I-7]$$

Equation [I-5] will be in the following form when the transformation of $r = e^{\theta}$ is made.

$$R(r) = C_1(1 + G_1 r + G_2 r^2 + \ldots$$
$$+ C_2(r + F_1 r^2 + F_2 r^3 \ldots$$

In order to satisfy the initial condition [I-6], C_1 must equal zero.

$$\frac{dR(r)}{dr} = C_2(1 + 2F_1 r + 3F_2 r^2 + \ldots)$$

Thus when $r = 0$ $\frac{dR(r)}{dr} = C_2$. The solution is thus some multiple of the slope. This multiple can be arbitrarily chosen. It is convenient to make the choice.

$$\frac{dR(r)}{dr} = 1, \quad r = 0$$

Thus $R(r) = e^{\theta} + F_1(0) e^{2\theta} + F_2(0) e^{3\theta} + \ldots$

It now remains to evaluate the coefficients.

To determine B, Q and T

Given: $\phi(0) = 1$ $\phi(1)$ and $\phi(2)$

Let the interval be h = 1/100 Bohr Units

The equation $B + Qr + Tr^2$ must be satisfied at the three given points and $B = 1$

$$\phi(1) = B + Qh + Th^2$$
$$\phi(2) = B + 2Qh + 4Th^2$$

and Q and T may be determined.

For each given value of E the values of BB, QQ and RR are determined.

To Evaluate the Coefficients

Operationally

$$\frac{1}{f(D)}e^{n\theta} = \frac{e^{n\theta}}{f(n)}$$

provided $D-n$ is not a factor of $f(D)$

If $D-n$ is a factor $\ni f(D) = (D-n)g(D)$

$$\rightarrow \frac{1}{f(D)}e^{n\theta} = \frac{e^{n\theta}}{(D-n)g(D)} = \frac{e^{n\theta}}{(D-n)g(n)} = \frac{(\theta-1)e^{n\theta}}{g(n)}$$

$\frac{1}{D-n}e^{n\theta}$ is the same as $(D-n)y = e^{n\theta}$

$$\begin{array}{rcl} D[(\theta-1)e^{n\theta}] & = & e^{n\theta}+n\theta e^{n\theta}-ne^{n\theta} \\ -n[(\theta-1)e^{n\theta}] & = & -n\theta e^{n\theta}+ne^{n\theta} \\ \hline (D-n)[(\theta-1)e^{n\theta}] & = & e^{n\theta} \end{array}$$

$$\frac{1}{D(D-1)}e^{n\theta} = \frac{1}{(D-1)(D-2)}e^{(n+1)\theta}$$

Thus, $F_1(D)e^{2\theta} = -\phi_1(D)e^{2\theta}$

$$= -\frac{BB}{D(D-1)}e^{2\theta}$$

$$= -\frac{BB}{2}e^{2\theta}$$

Let $-\frac{BB}{2} = F_1(2)$

Similarly,

$$F_2(D)e^{3\theta} = -(\phi_1(D)F_1(D-1) + \phi_2(D))e^{3\theta}$$

$$F_1(D-1)e^{3\theta} = F_1(D)e^{2\theta}$$

$$F_1(D-1) = F_1(2)$$

$$\rightarrow F_2(D)e^{3\theta} = -\left(\frac{BB}{D(D-1)}F_1(2) - \frac{QQ}{D(D-1)}\right)e^{3\theta}$$

Let $$-\frac{1}{3\cdot 2}(-BB\,F_1(2) - QQ) = F_2(3)$$

$$F_3(D)e^{4\theta} = -(\phi_1(D)F_2(D-1) - \phi_2(D)F_1(D-2) - \phi_3(D))e^{4\theta}$$

$$= -\left(\frac{BB}{D(D-1)}F_2(3) - \frac{QQ}{D(D-1)}F_1(2) - \frac{RR}{D(D-1)}\right)e^{4\theta}$$

Let $$-\frac{1}{4\cdot 3}\left(BB\,F_2(3) - QQ\,F_1(2) - RR\right) = F_3(4)$$

$$F_4(D)e^{5\theta} = -\left(\frac{BB}{D(D-1)}F_3(4) - \frac{QQ}{D(D-1)}F_2(3) - \frac{RR}{D(D-1)}F_1(2)\right)e^{5\theta}$$

Let $$-\frac{1}{5\cdot 4}\left(BB\,F_3(4) - QQ\,F_2(3) - RR\,F_1(2)\right) = F_4(5)$$

In general

$$F_n(n+1) = -\frac{1}{n(n-1)}\left\{BB\,F_{n-1}(n-1) + QQ\,F_{n-2}(n-2) + RR\,F_{n-3}(n-3)\right\}$$

This type of recursion formula is easily put in FORTRAN language and the number of coefficients that can be calculated is unlimited.

Using the notation $F_n(n+1) = F_n$

$$R(r) = e^{\theta} + F_1 e^{2\theta} + F_2 e^{3\theta} + \cdots + F_n e^{(n+1)\theta}$$

or since $r = e^{\theta}$ the equation becomes

$$R(r) = r + F_1 r^2 + F_2 r^3 + F_3 r^3 + \cdots + F_n r^{n+1} \qquad [\text{I-8}]$$

This equation is easily summed in FORTRAN language. The convergence is most easily observed by calculating the partial sums. For the initial calculation with h = .01 it was observed that ten terms were sufficient to reach the limit of the machine 10^{-307}. Equation [I-8] was used to compute the starting values of all computations.

The Case When the Initial Conditions Are:

$$R(r) = R(k) \qquad r = k$$
$$\frac{dR(r)}{dr} = R'(k) \qquad r = k$$

The form of the equations will be

$$R(r) = C_1\left(1 + G_1 r + G_2 r^2 + \cdots G_n r^n\right) + C_2\left(r + F_1 r^2 + F_2 r^3 + \cdots + F_n r^{n+1}\right)$$

$$\frac{dR(r)}{dr} = C_1\left(G_1 + 2G_2 r + 3G_3 r^2 + \cdots + nG_n r^{n-1}\right) + C_1\left(r\frac{dG_1}{dr} + r^2\frac{dG_2}{dr} + \cdots + r^n\frac{dG_n}{dr}\right) + C_2\left(1 + 2F_1 r + 3F_2 r^2 + \cdots n{+}1\, F_n r^n\right)$$

It will be shown that G_i is a function of r and F_i is a constant.

At any coordinate $r=k$ if $G_i, \frac{dG_i}{dr}$ and F_i are determined.

Then
$$R(k) = C_1 g_1(k) + C_2 f_1(k)$$
$$R'(k) = C_1 g_2(k) + C_2 f_2(k)$$

Thus C_1 and C_2 are determined.

For the portion

$$R(r) = C_2 (e^{\theta} + F_1(D) e^{2\theta} + \dots F_n(D) e^{(n+1)\theta})$$

the solution is exactly the same as the starting case.

For

$$R(r) = C_1 (1 + G_1(D) e^{\theta} + G_2(D) e^{2\theta} + \dots G_n(D) e^{n\theta})$$

the calculation is more complex.

$$\begin{aligned} F_1(D) e^{\theta} &= -\phi_1(D) e^{\theta} \\ &= -\frac{BB}{D(D-1)} e^{\theta} \\ &= -BB(\theta - 1) e^{\theta} \end{aligned}$$

Now change to the following rather complex notation. This notation will be needed later when derivatives are taken.

Since $r = e^{\theta}$ $\theta = \ln r$

Let
$$V(1) = -BB$$
$$AC(1) = V(1)$$
$$VV(1) = BB$$
$$BC(1) = VV(1)$$
$$G(1) = AC(1)\theta + BC(1)$$

Then $F_1(D)e^{\theta} = G(1)e^{\theta}$

$$\frac{1}{D(D-1)}\theta e^{n\theta} = e^{n\theta}\left\{\frac{1}{(n+D)(D+n-1)}\theta\right\}$$

$$(D+n)(D+n-1) = D^2+(2n-1)D+n(n-1)$$

$$= n(n-1)\left\{1+\frac{2n-1}{n(n-1)}D+\frac{D^2}{n(n+1)}\right\}$$

Since $D^2\theta = 0$ dividing the remainder into one,

$$1+\frac{2n-1}{n(n-1)}D\,\overline{\big)\,1} \quad = 1-\frac{2n-1}{n(n-1)}D$$

Thus $\frac{1}{D(D-1)}\theta e^{n\theta} = e^{n\theta}\left\{\frac{1}{n(n-1)}-\frac{(2n-1)}{(n[n-1])^2}D\right\}\theta$

$$= \frac{e^{n\theta}}{n(n-1)}\left\{\theta-\frac{2n-1}{n(n-1)}\right\} \quad n\geq 2$$

Evaluating $F_2(D)$

$$F_2(D)e^{2\theta} = -\phi_1(D)F_1(D-1)e^{2\theta}-\phi_2(D)e^{2\theta}$$

$$= -\frac{BB}{D(D-1)}AC(1)\theta e^{2\theta}-\frac{BB}{D(D-1)}BC(1)e^{2\theta}-\frac{QQ}{D(D-1)}e^{2\theta}$$

$$= -\left(\frac{BB}{2}\left(\theta-\frac{3}{2}\right)AC(1)+\frac{BB}{2}BC(1)+\frac{QQ}{2}\right)e^{2\theta}$$

$V(2) = -\frac{BB\cdot AC(1)}{2}$ $\qquad VV(2) = -\frac{BB}{2}\left(BC(1)-\frac{3}{2}AC(1)\right)$

$WW(2) = -\frac{QQ}{2}$

$AC(2) = V(2)$ $\qquad BC(2) = VV(2)+WW(2)$

$$G(2) = AC(2)\theta+BC(2)$$

Proceeding in like manner for $F_3(D)$

$$V(3) = -\frac{BB}{6}AC(2) \qquad VV(3) = -\frac{1}{6}\left\{\frac{5BB}{6}\cdot AC(2) + BC(2)\right\}$$

$$W(3) = -\frac{QQ}{6}AC(1) \qquad WW(3) = -\frac{1}{6}\left\{\frac{5QQ}{6}\cdot AC(1) + BC(1)\right\}$$

$$XX(3) = -\frac{1}{6}\cdot RR$$

$$AC(3) = V(3) + W(3) \qquad BC(3) = VV(3) + WW(3) + XX(3)$$

$$G(3) = AC(3)\cdot\theta + BC(3)$$

The General Term becomes

$$V(J) = -\frac{1}{J(J+1)}\left(BB\cdot AC(J-1)\right)$$

$$W(J) = -\frac{1}{J(J+1)}\left(QQ\cdot AC(J-2)\right)$$

$$X(J) = -\frac{1}{J(J+1)}\left(RR\cdot AC(J-3)\right)$$

$$VV(J) = -\frac{1}{J(J+1)}\left(BB\cdot AC(J-1)\left(\frac{2J-1}{J(J-1)}\right) + BC(J-1)\right)$$

$$WW(J) = -\frac{1}{J(J+1)}\left(QQ\cdot AC(J-2)\left(\frac{2J-1}{J(J-1)}\right) + BC(J-2)\right)$$

$$XX(J) = -\frac{1}{J(J+1)}\left(RR\cdot AC(J-3)\left(\frac{2J-1}{J(J-1)}\right) + BC(J-3)\right)$$

$$AC(J) = V(J) + W(J) + X(J)$$

$$BC(J) = VV(J) + WW(J) + XX(J)$$

$$G(J) = AC(J)\cdot\theta + BC(J)$$

For example

$$G(4) = AC(4)\cdot\theta + BC(4)$$

$$BC(4) = VV(4) + WW(4) + XX(4)$$

Thus $VV(4) = -\frac{1}{4\cdot 3}\left(BB\cdot AC(3)\cdot\frac{7}{12} + BC(3)\right)$

Therefore the form of the equation will be

$$R(r) = C_1(1 + G_1 e^{\theta} + G_2 e^{2\theta} + --- + G_n e^{n\theta})$$

since $r = e^{\theta}$; $G(i) = AC(i)\theta + BC(i) = AC(i)\cdot\ln r + BC(i)$

$$R(r) = C_1(1 + \ln r\,[AC(1)\cdot r + AC(2)\cdot r^2 + \ldots])$$

$$+ C_1(BC(1)\cdot r + BC(2)\cdot r^2 + BC(3)\cdot r^3 + \ldots)$$

and the complete solution is

$$\begin{aligned} R(r) = {} & C_1(1 + \ln r\,[AC(1)\cdot r + AC(2)\cdot r^2 + ---] \\ & + C_1(BC(1)\cdot r + BC(2)\cdot r^2 + ---) \\ & + C_2(r + F_1 r^2 + F_2 r^3 + ---) \end{aligned}$$

$$\begin{aligned} \frac{dR(r)}{dr} = {} & C_1\left\{\frac{1}{r}(AC(1)\cdot r + AC(2)\cdot r^2 + --- AC(n)\cdot r^n\right\} \\ & + C_1\left\{\ln r\,(AC(1) + 2AC(2)\cdot r + --- nAC(n)r^{n-1})\right\} \\ & + C_1\left\{BC(1) + 2BC(2)\cdot r + --- nBC(n)r^{n-1}\right\} \\ & + C_2\left\{1 + 2F_1 r + 3F_2 r^2 + --- nF_{n-1} r^{n-1}\right\} \end{aligned}$$

A similar expression can be derived for the second derivative.

Discussion of the Equation

The equation of R(r) is slowly converging. The second derivative is more slowly converging. The self-checking feature is obtained by comparing the second derivative with the value of the second derivative calculated from

$$\frac{d^2R}{dr^2} = f(r)R$$

It was observed that 10 terms of the series were sufficient to tax the limit of machine accuracy for the starting values. When r = 1 the number of terms required is 25, 50 for r = 3, and 75 for r = 8.

The number of calculations required to carry out the series to 75 terms is fantastic. One run required 20 minutes of machine time. In order to determine the lowest energy state and to properly determine the points of tangency, increments of .001 E were used. Thus it would take approximately 30 machine hours to complete one Wigner-Seitz calculation using this method.

Even though the 75th coefficient time $(8)^{75}$ was of the order of 10^{-200} the build-up errors encountered because of the large number of calculations allowed agreement on the check to only 10^{-8}.

The equation did, however, serve its purpose and enabled us to establish a criterion. Fortunately the simplest formula used

$$R(r+\Delta r) = (2 - (\delta r)^2 f(r))R(r) - R(r-\Delta r)$$

using an interval of .01 Bohr units duplicated the results of the very complex system described above to 10^{-6}. The Wigner-Seitz calculation by this method takes approximately 5 to 10 minutes of machine time compared with 30 hours for the complex method.

APPENDIX II

THE RADIAL WAVE FUNCTIONS R(r) FOR ENERGIES RANGING FROM THE IONIZATION ENERGY TO THE LOWEST ENERGY STATE FOR COPPER, SILVER, AND GOLD.

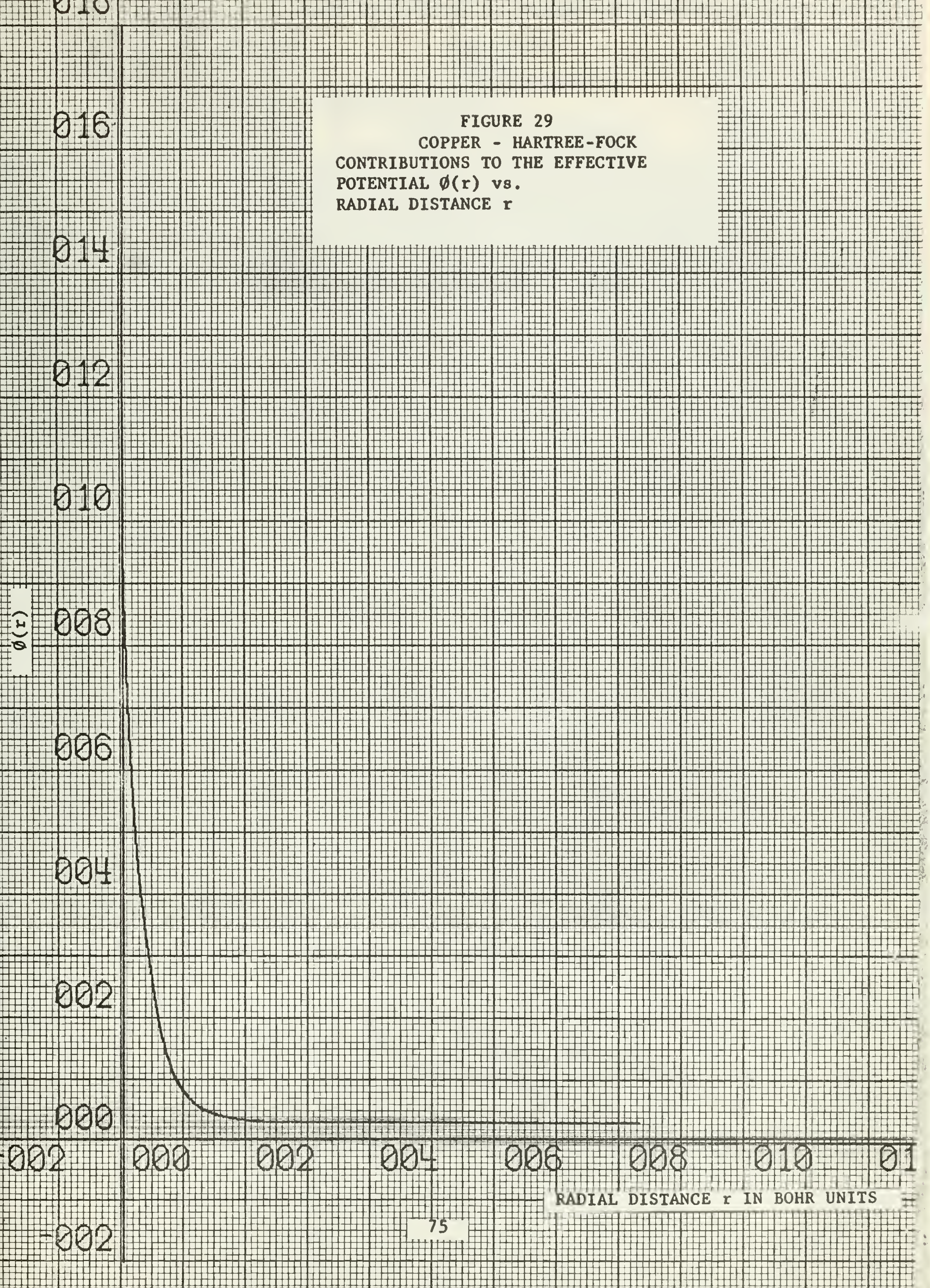


FIGURE 29
COPPER - HARTREE-FOCK
CONTRIBUTIONS TO THE EFFECTIVE
POTENTIAL Ø(r) vs.
RADIAL DISTANCE r

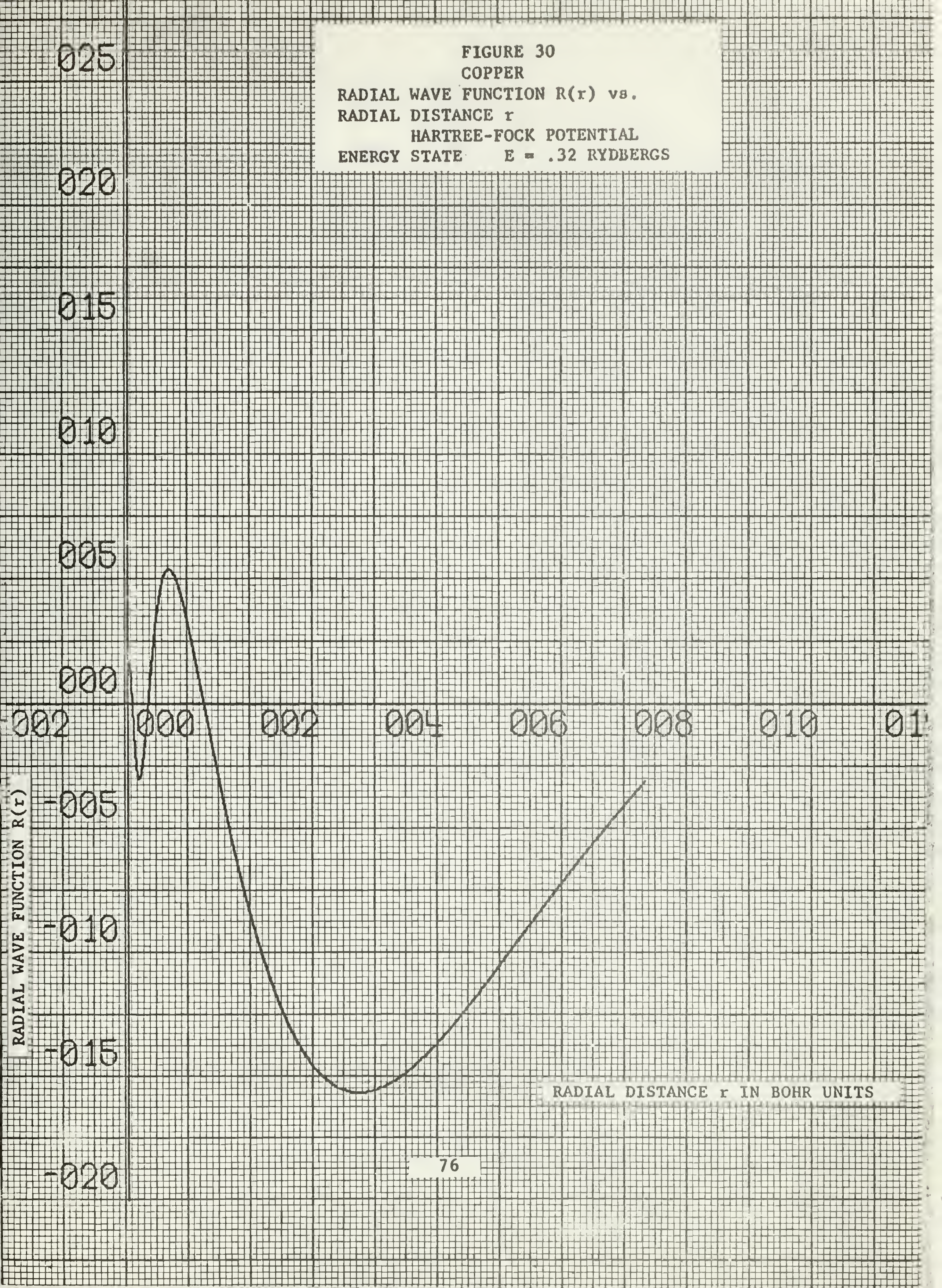


FIGURE 30
COPPER
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
HARTREE-FOCK POTENTIAL
ENERGY STATE E = .32 RYDBERGS

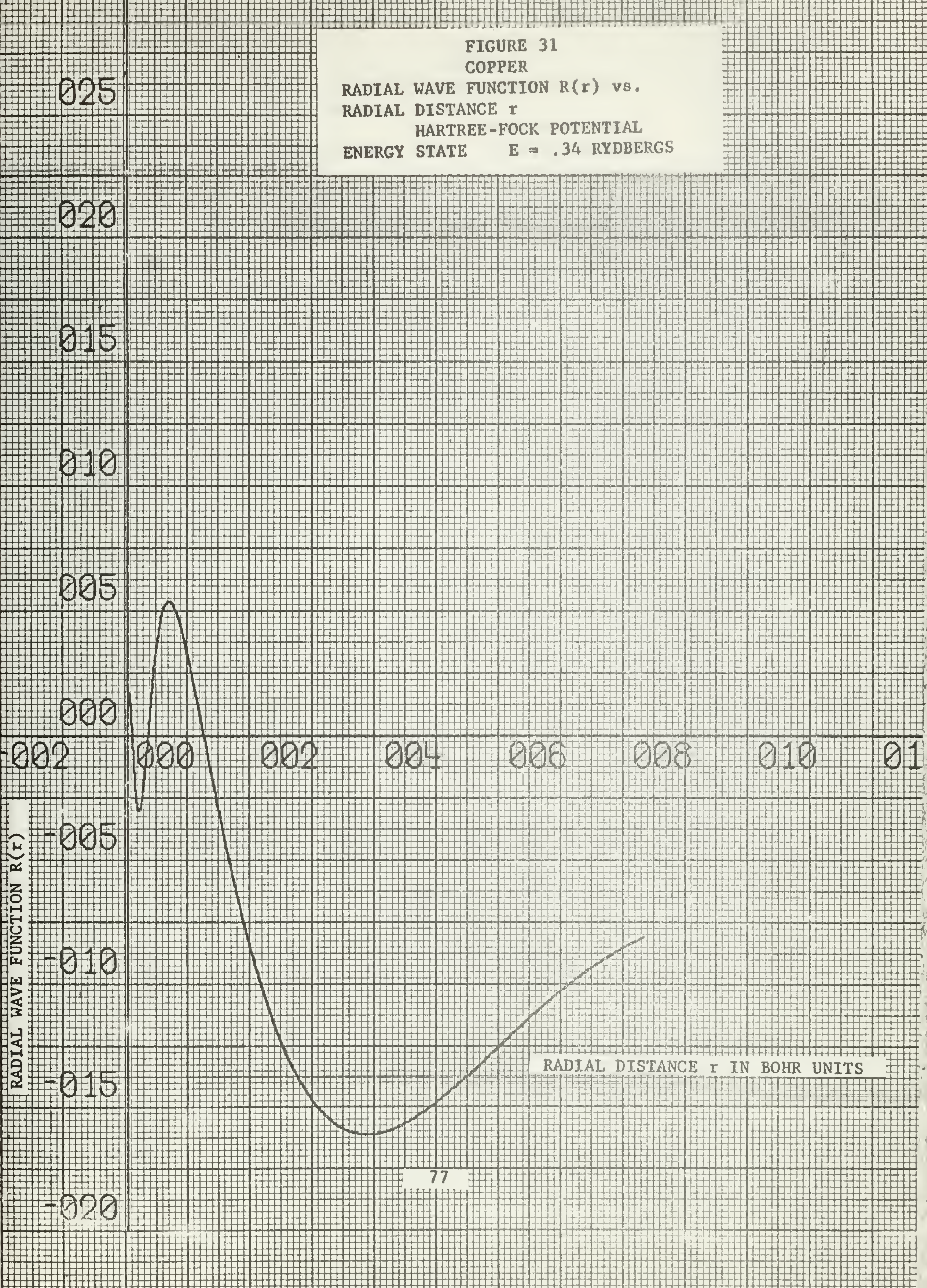


FIGURE 31
COPPER
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
HARTREE-FOCK POTENTIAL
ENERGY STATE E = .34 RYDBERGS

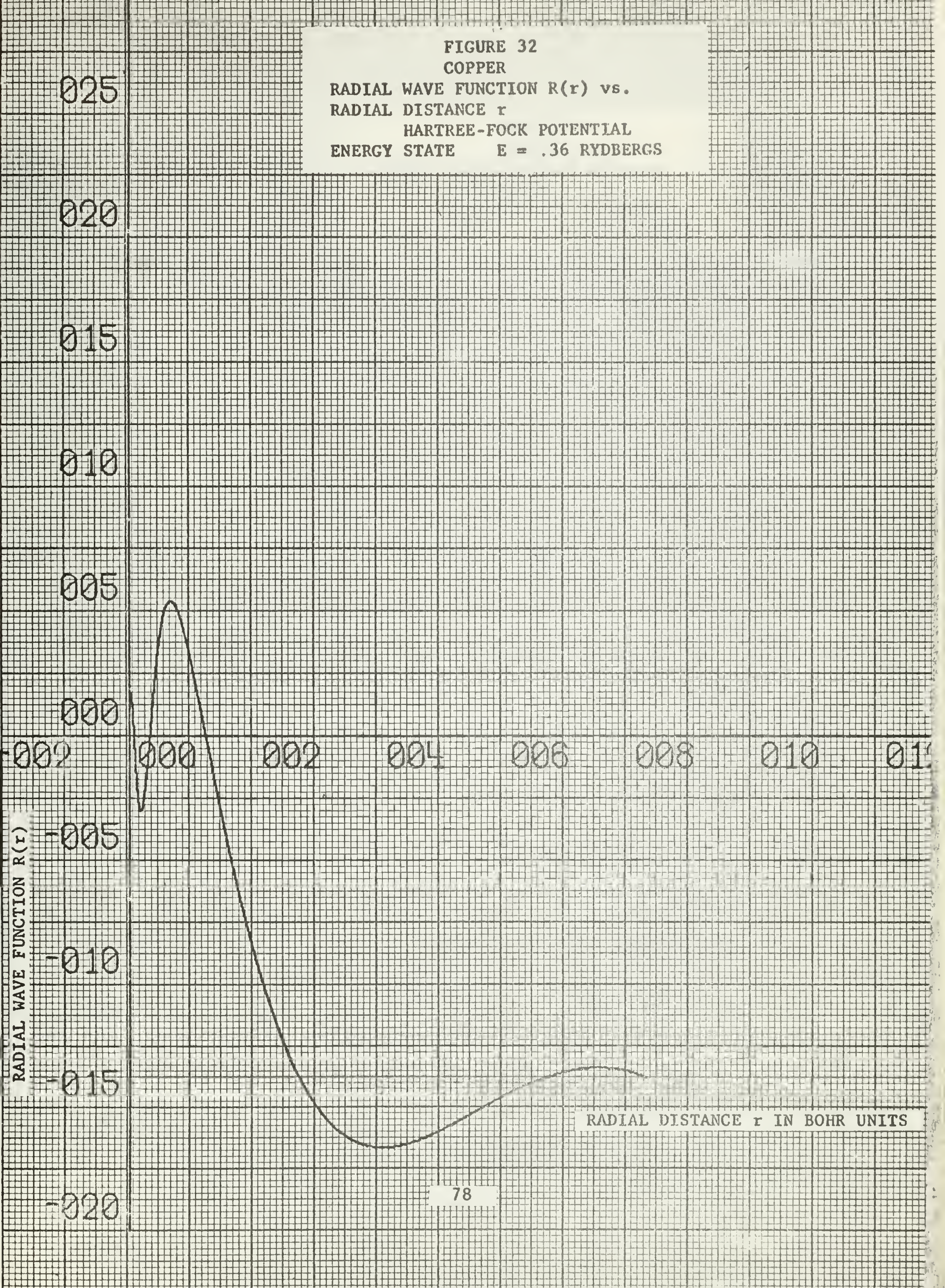


FIGURE 32
COPPER
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
HARTREE-FOCK POTENTIAL
ENERGY STATE E = .36 RYDBERGS

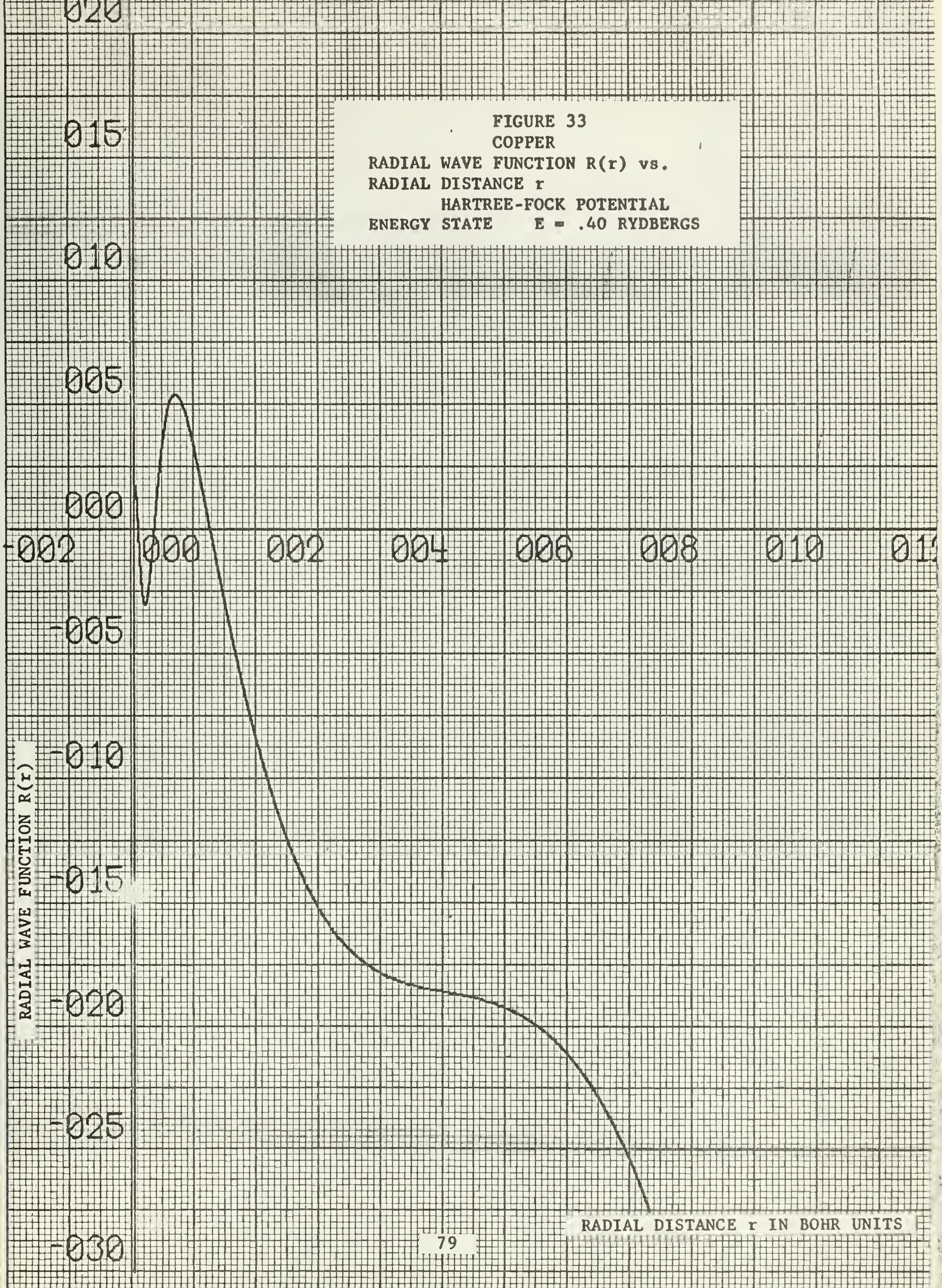


FIGURE 33
COPPER
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
HARTREE-FOCK POTENTIAL
ENERGY STATE E = .40 RYDBERGS

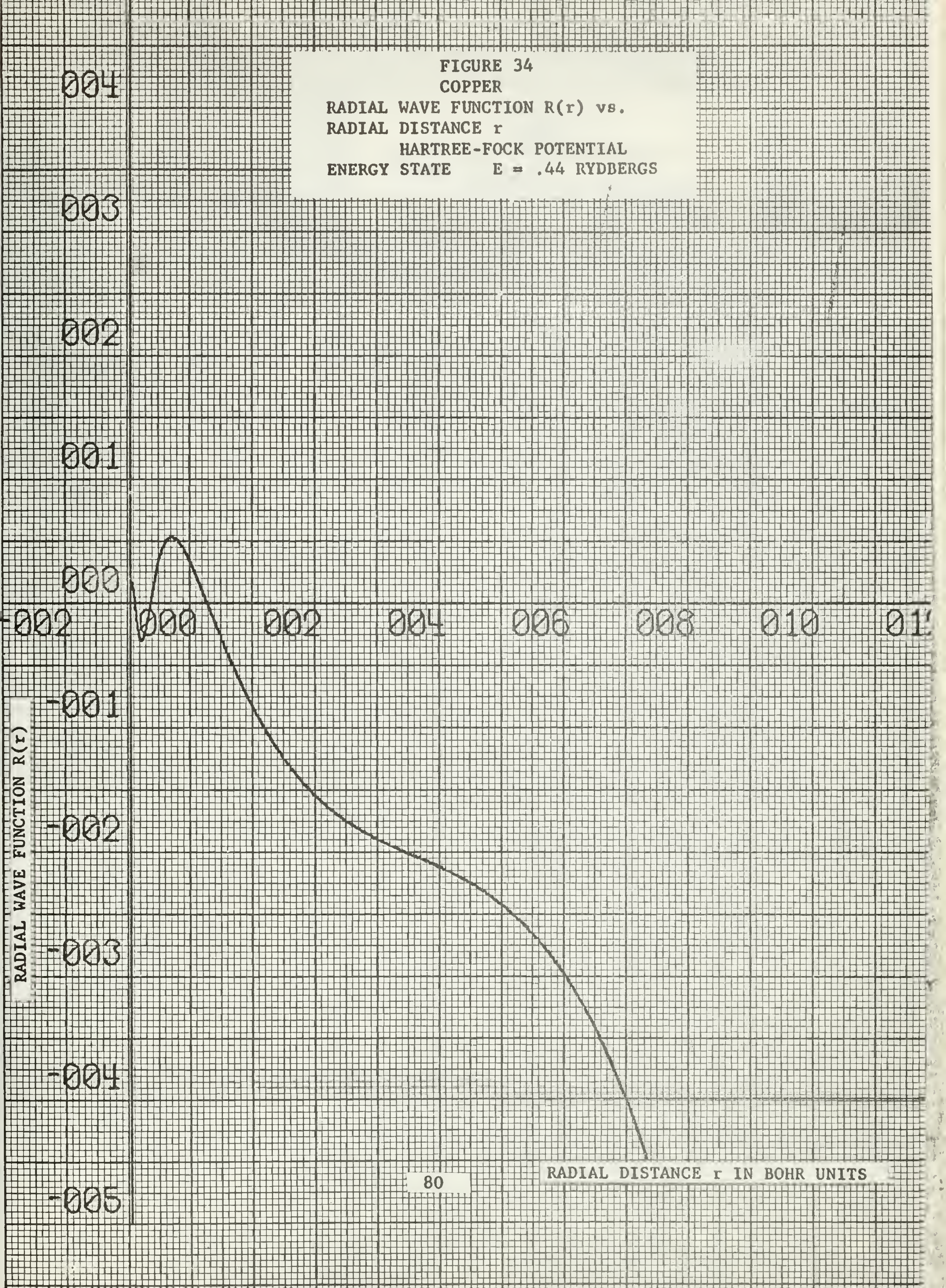


FIGURE 34
COPPER
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
HARTREE-FOCK POTENTIAL
ENERGY STATE E = .44 RYDBERGS

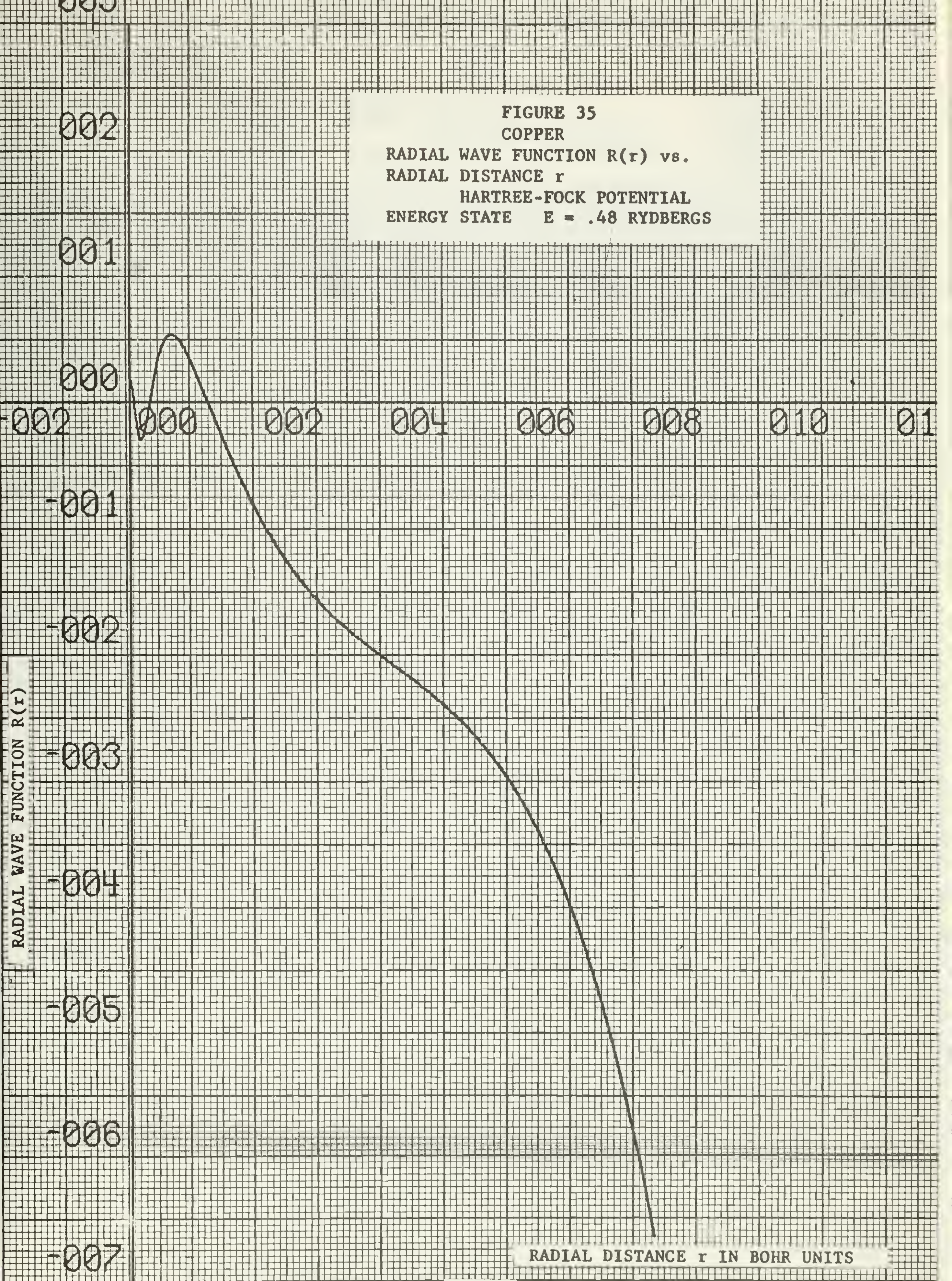


FIGURE 35
COPPER
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
HARTREE-FOCK POTENTIAL
ENERGY STATE E = .48 RYDBERGS

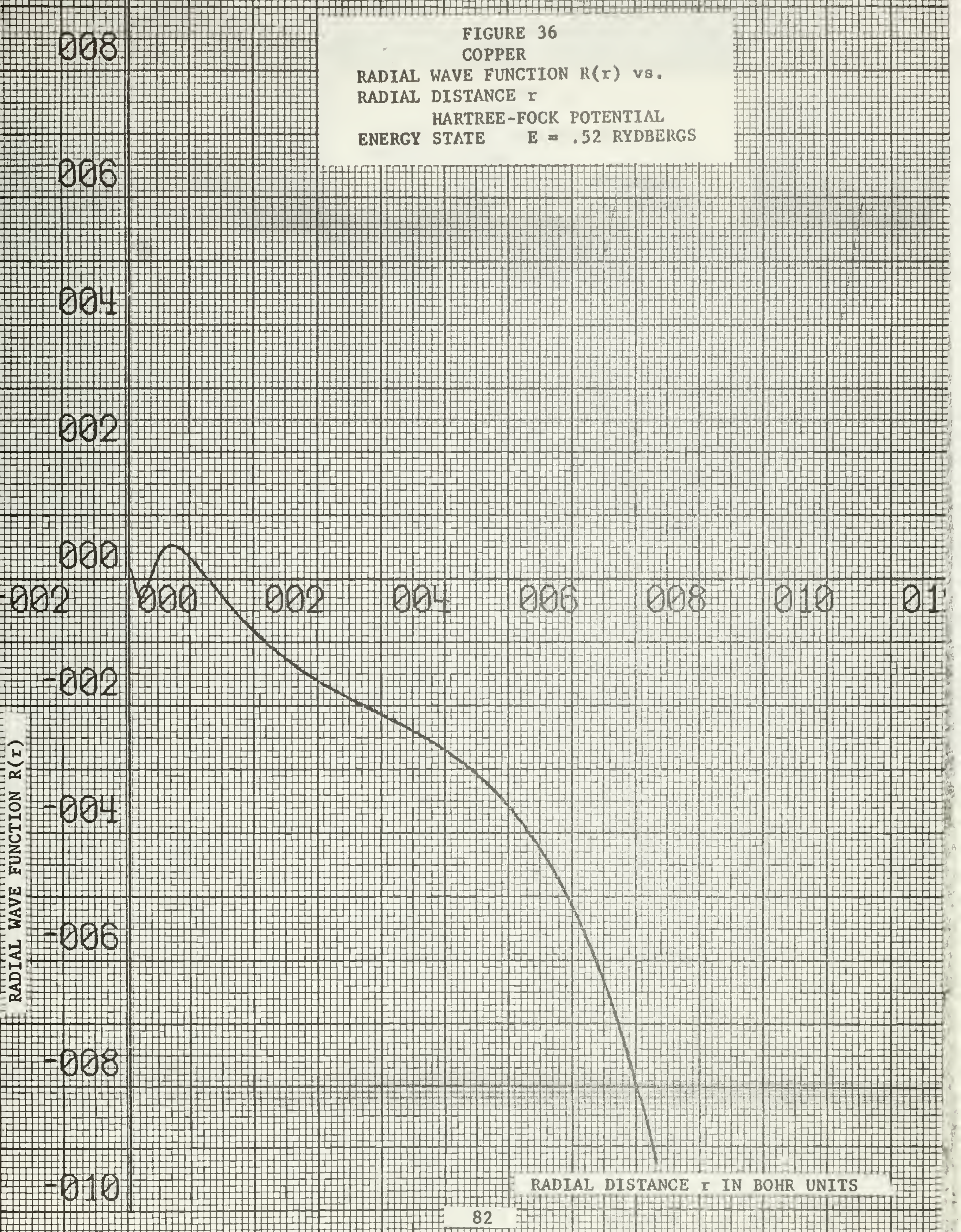


FIGURE 36
COPPER
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
HARTREE-FOCK POTENTIAL
ENERGY STATE E = .52 RYDBERGS

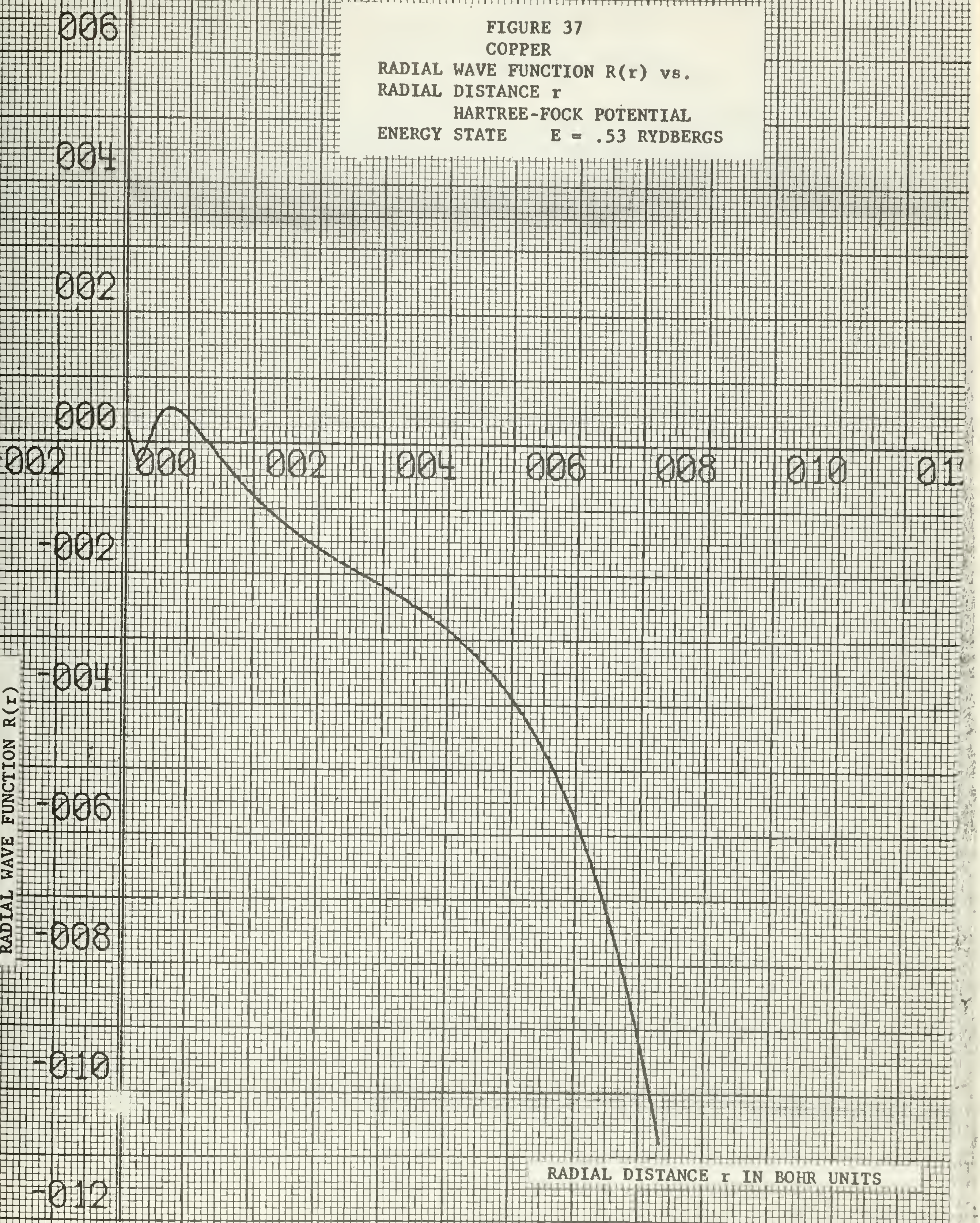


FIGURE 37
COPPER
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
HARTREE-FOCK POTENTIAL
ENERGY STATE E = .53 RYDBERGS

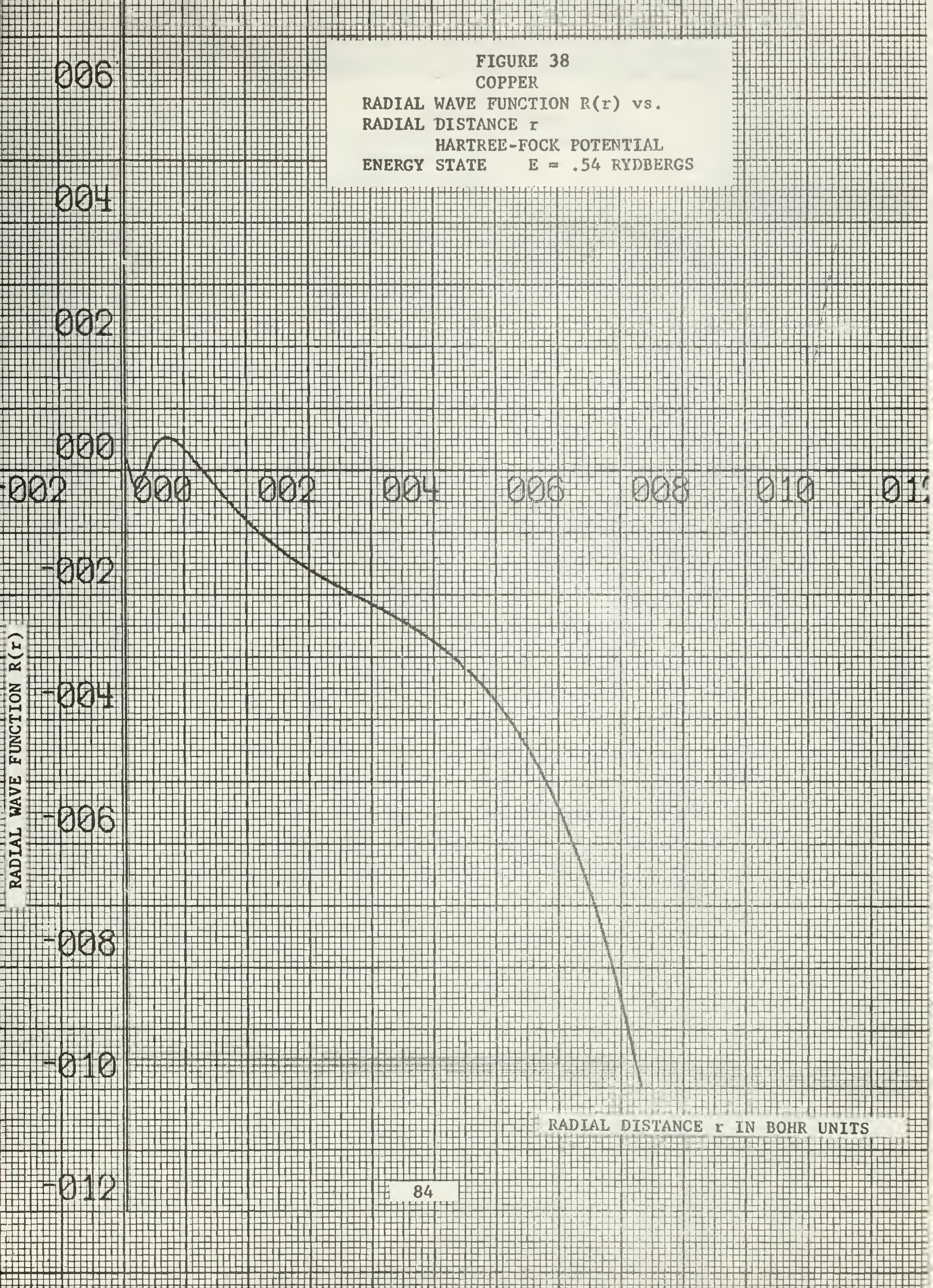


FIGURE 38
COPPER
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
HARTREE-FOCK POTENTIAL
ENERGY STATE E = .54 RYDBERGS

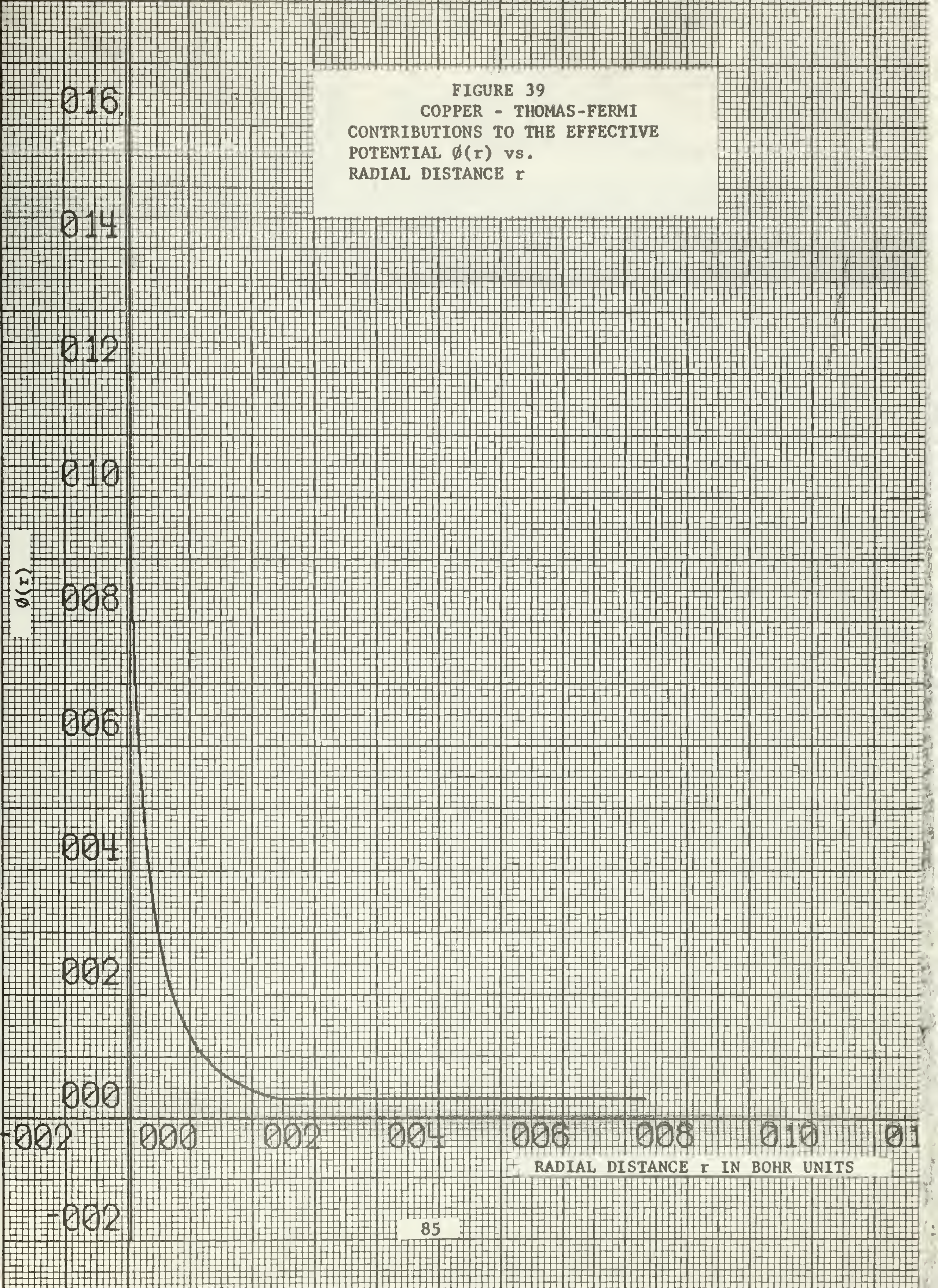


FIGURE 39
COPPER - THOMAS-FERMI
CONTRIBUTIONS TO THE EFFECTIVE
POTENTIAL ø(r) vs.
RADIAL DISTANCE r

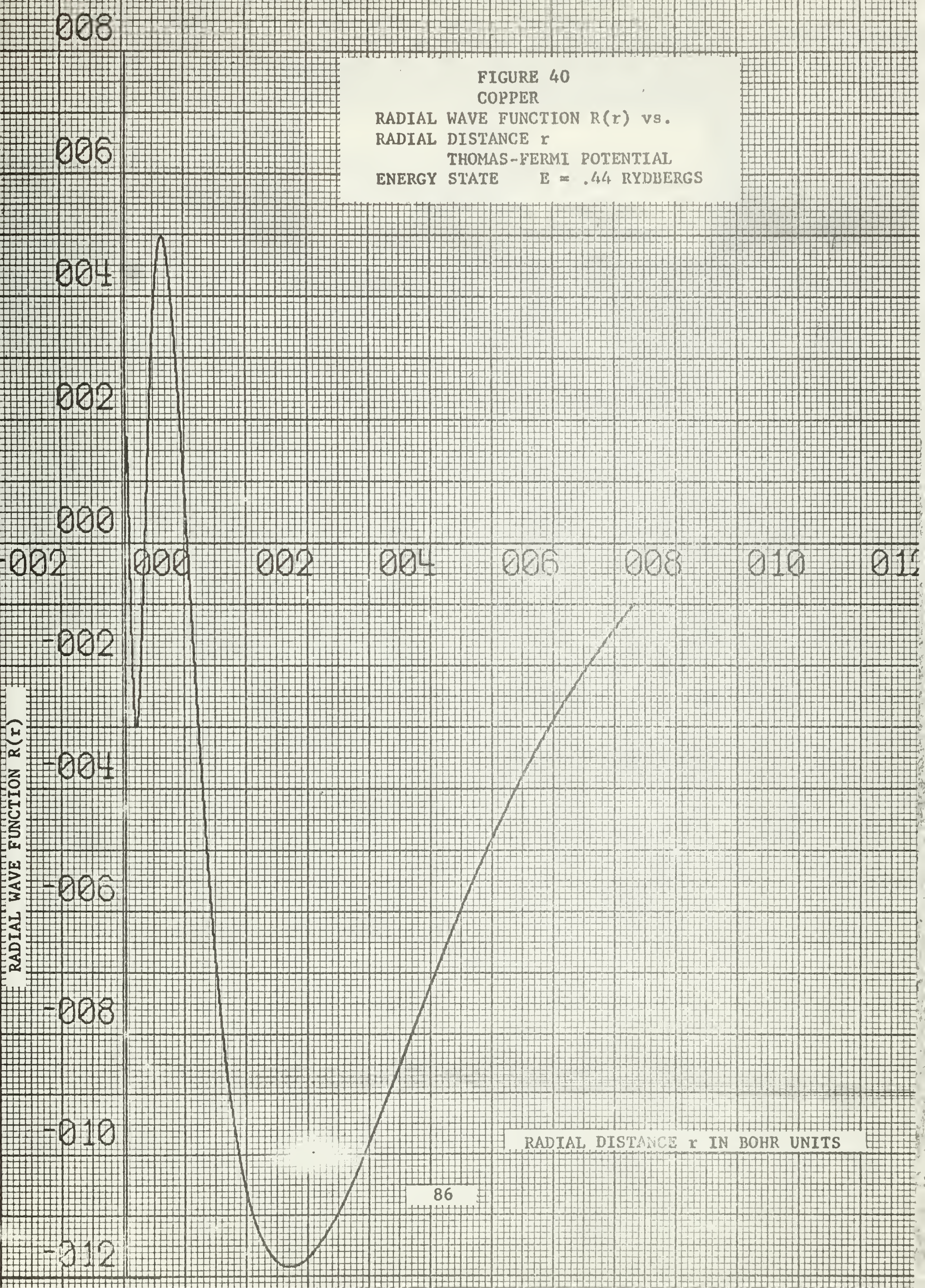


FIGURE 40
COPPER
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
THOMAS-FERMI POTENTIAL
ENERGY STATE E = .44 RYDBERGS

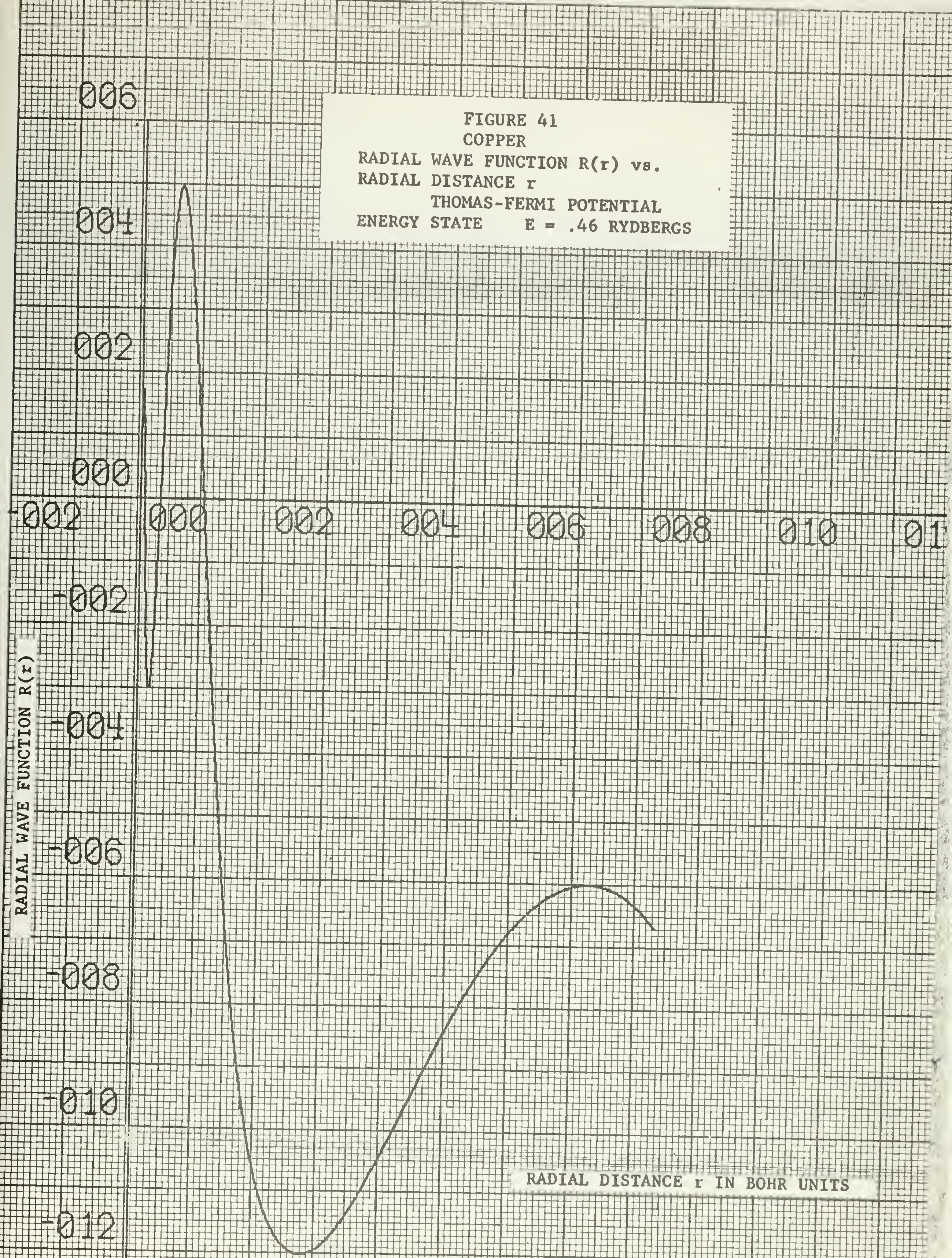


FIGURE 41
COPPER
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
THOMAS-FERMI POTENTIAL
ENERGY STATE E = .46 RYDBERGS

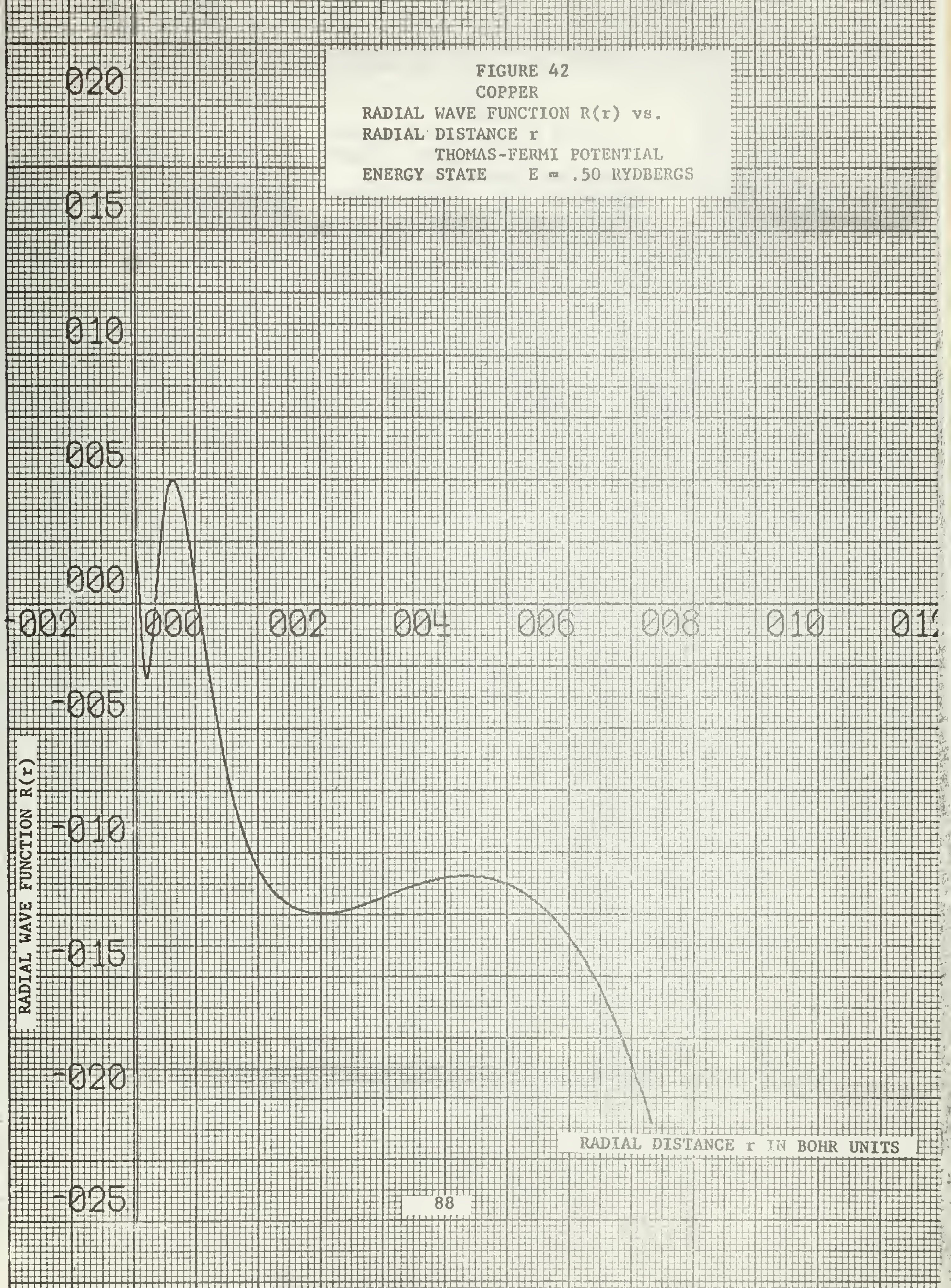


FIGURE 42
COPPER
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
THOMAS-FERMI POTENTIAL
ENERGY STATE E = .50 RYDBERGS

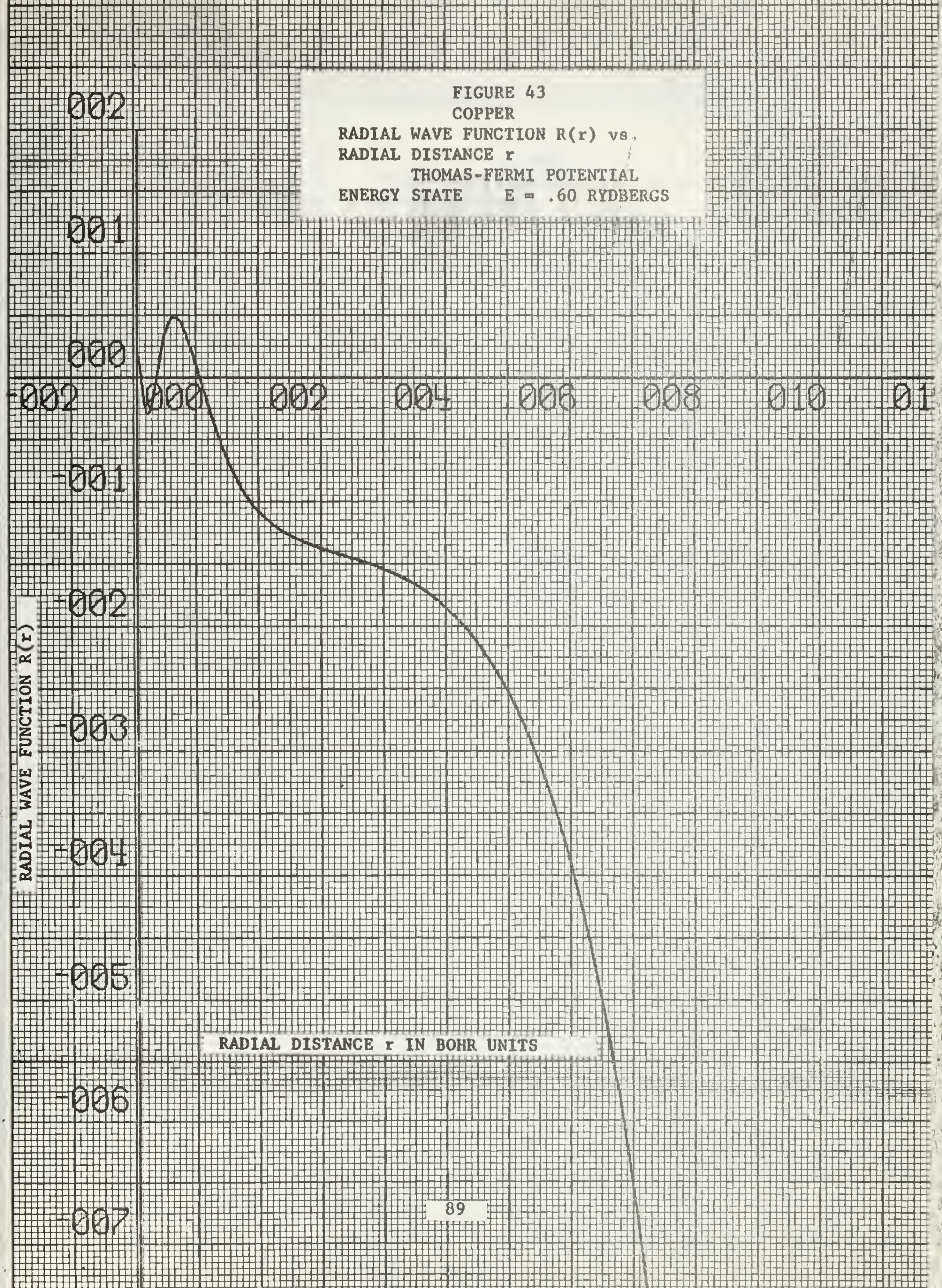


FIGURE 43
COPPER
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
THOMAS-FERMI POTENTIAL
ENERGY STATE E = .60 RYDBERGS

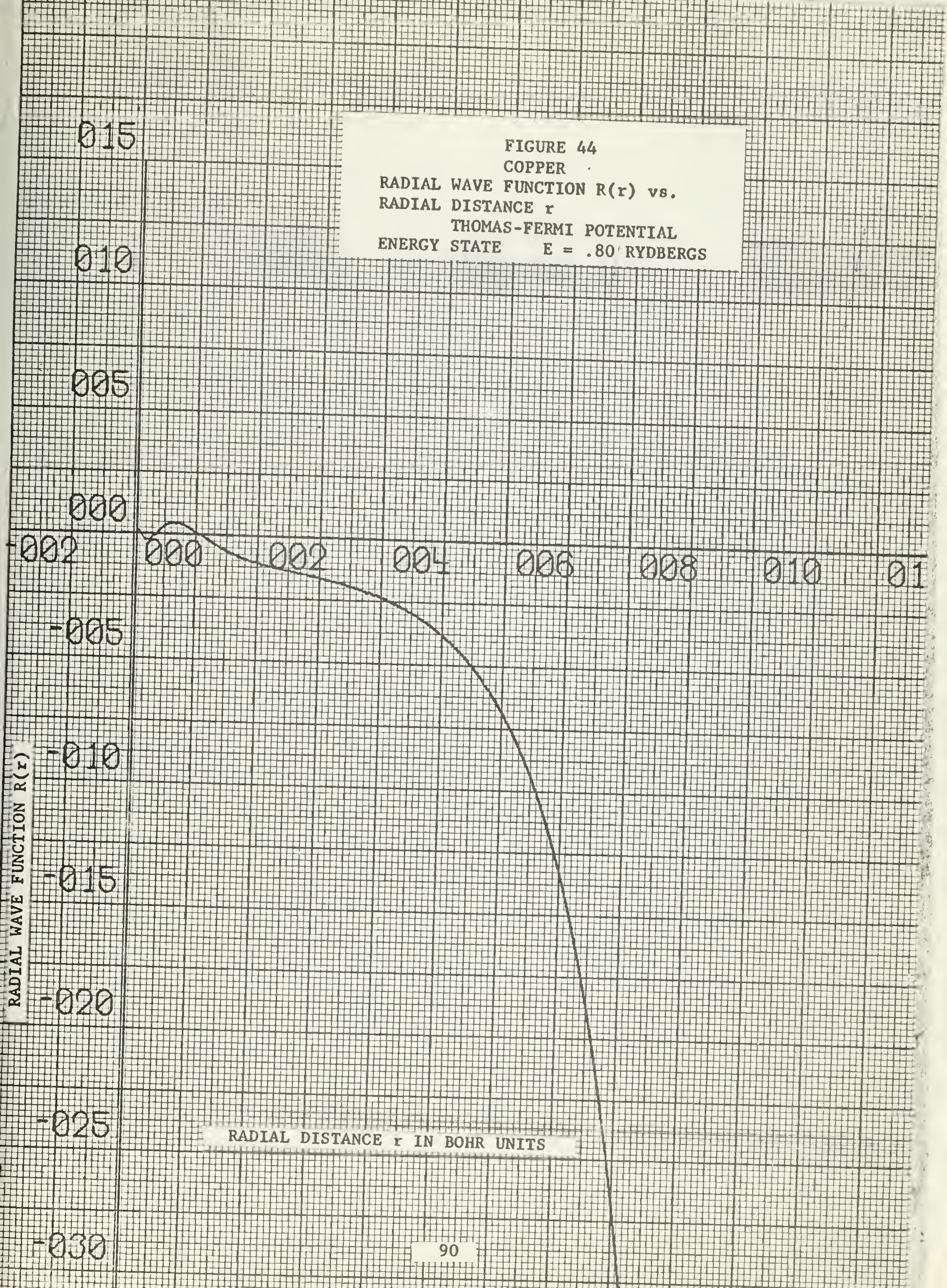
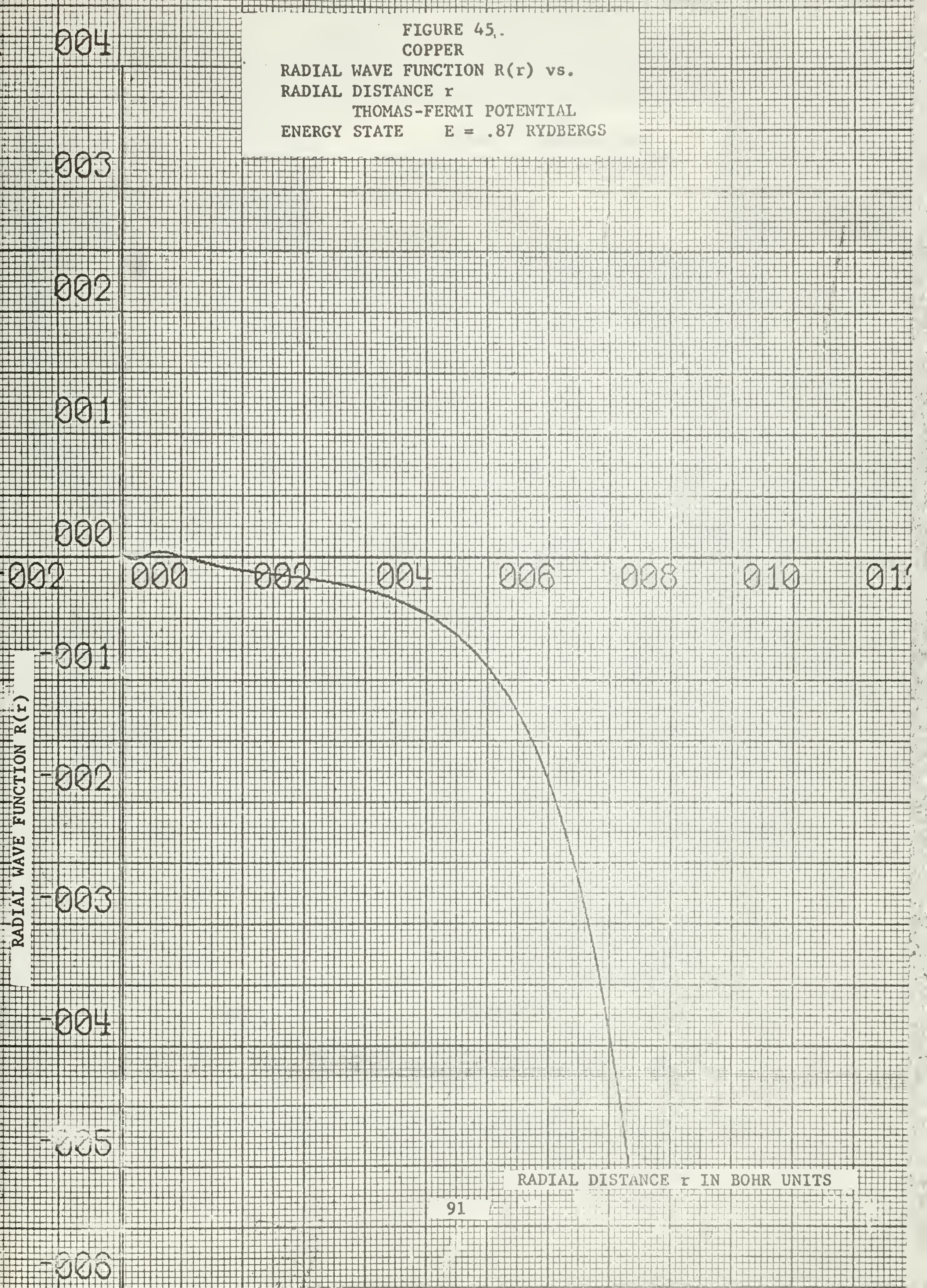


FIGURE 44
COPPER
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
THOMAS-FERMI POTENTIAL
ENERGY STATE E = .80 RYDBERGS

FIGURE 45.
COPPER
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
THOMAS-FERMI POTENTIAL
ENERGY STATE E = .87 RYDBERGS



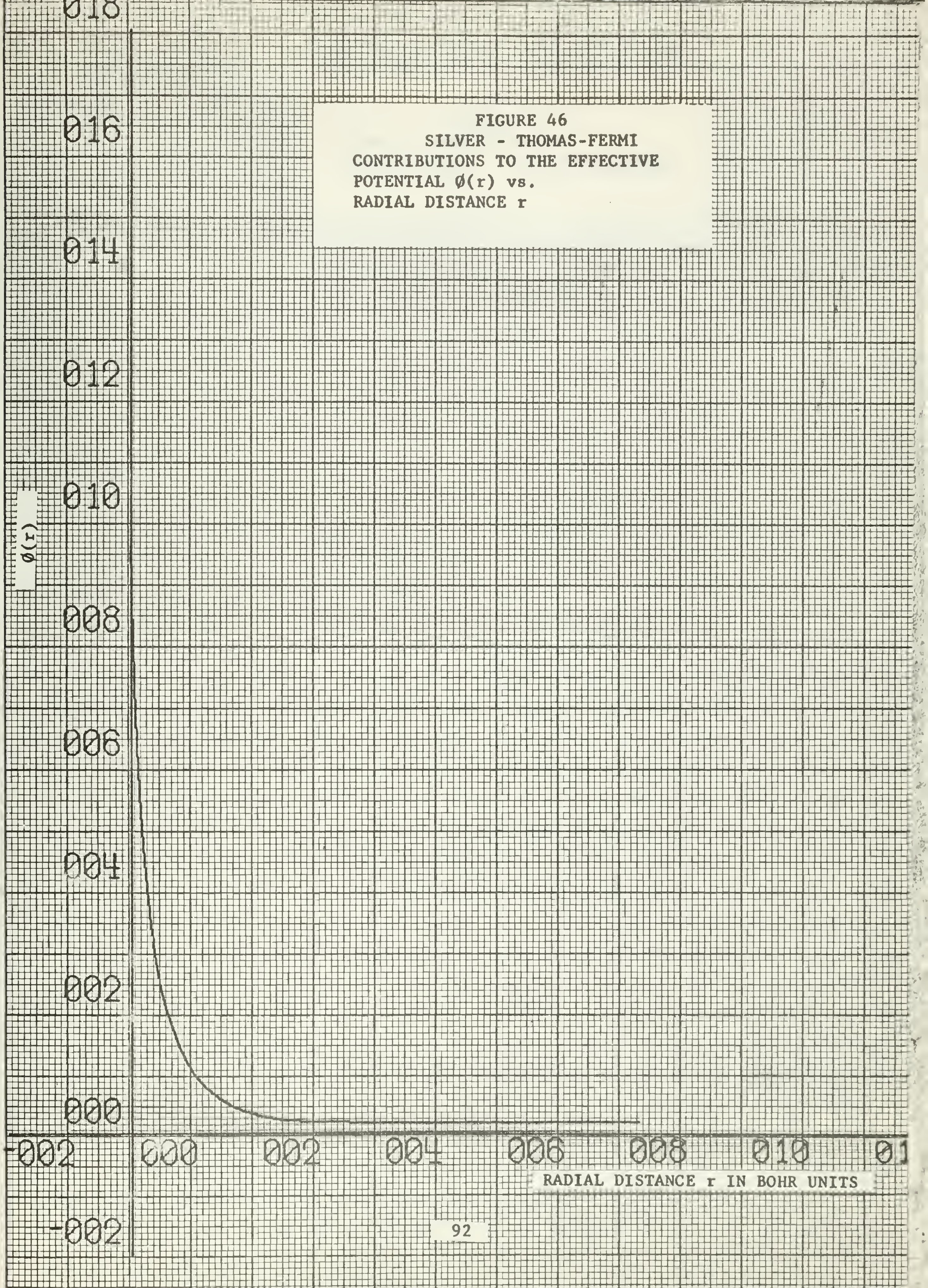


FIGURE 46
SILVER - THOMAS-FERMI
CONTRIBUTIONS TO THE EFFECTIVE
POTENTIAL Ø(r) vs.
RADIAL DISTANCE r

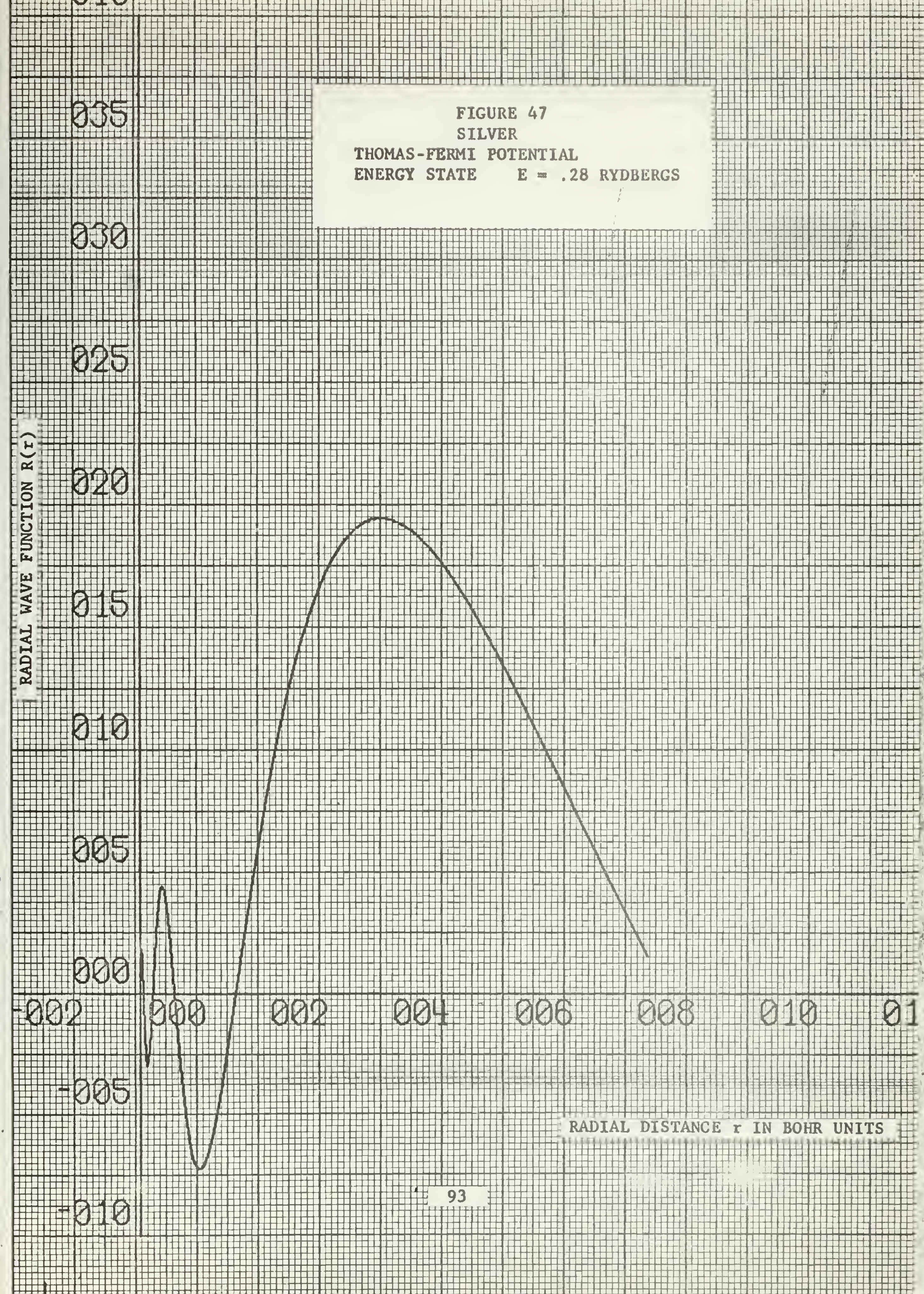


FIGURE 47
SILVER
THOMAS-FERMI POTENTIAL
ENERGY STATE E = .28 RYDBERGS

[illegible]

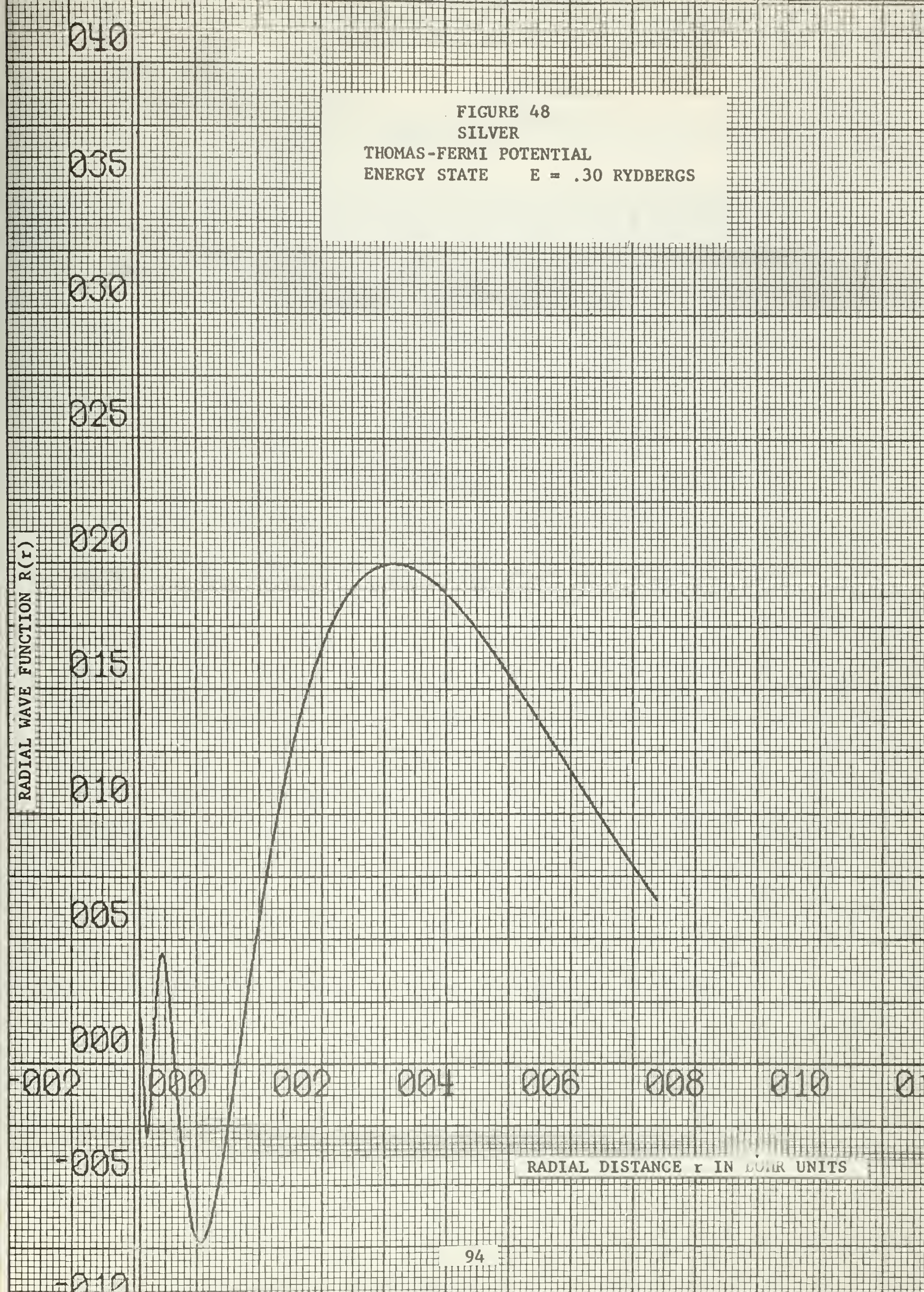


FIGURE 48
SILVER
THOMAS-FERMI POTENTIAL
ENERGY STATE E = .30 RYDBERGS

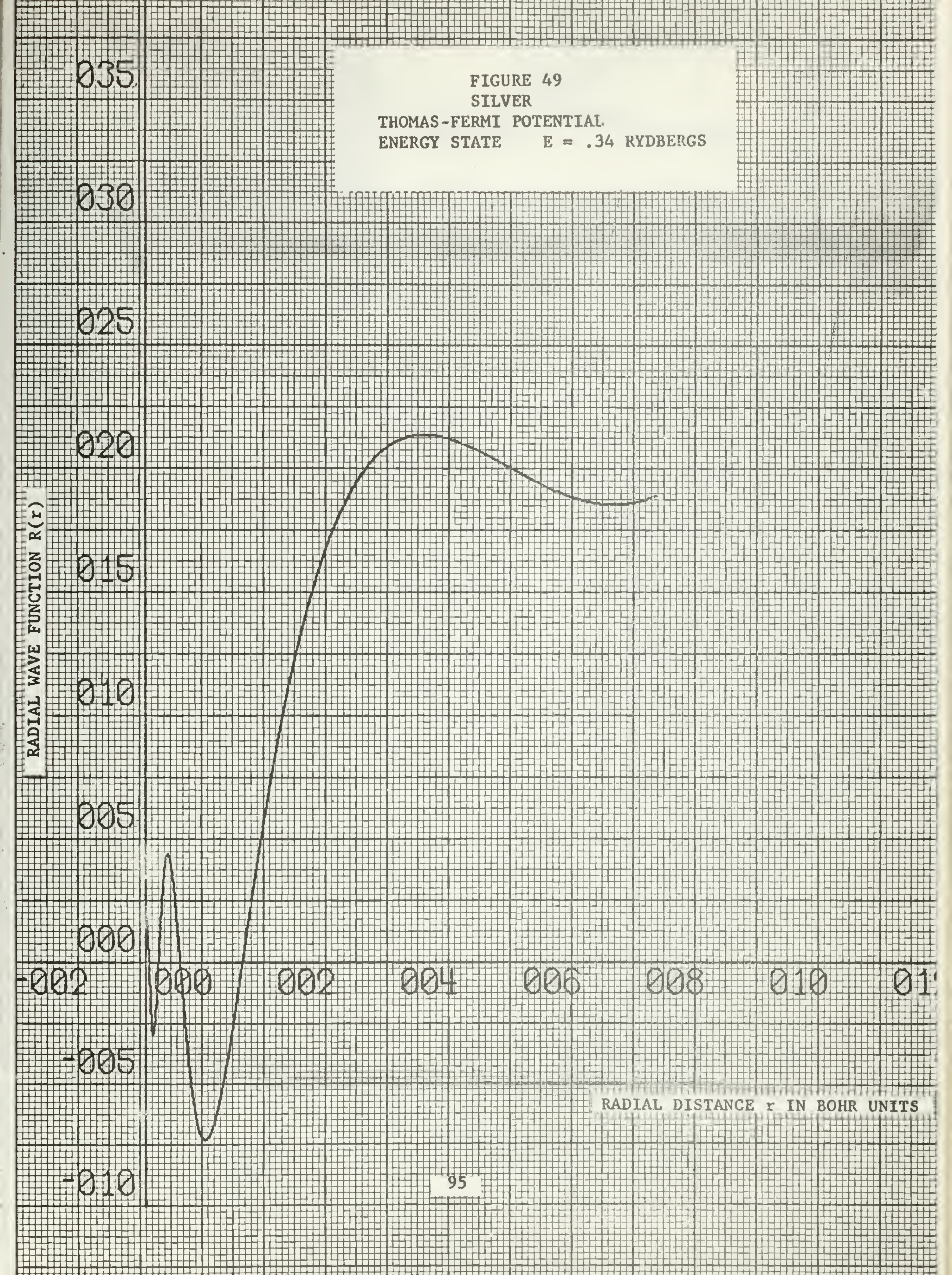


FIGURE 49
SILVER
THOMAS-FERMI POTENTIAL
ENERGY STATE E = .34 RYDBERGS

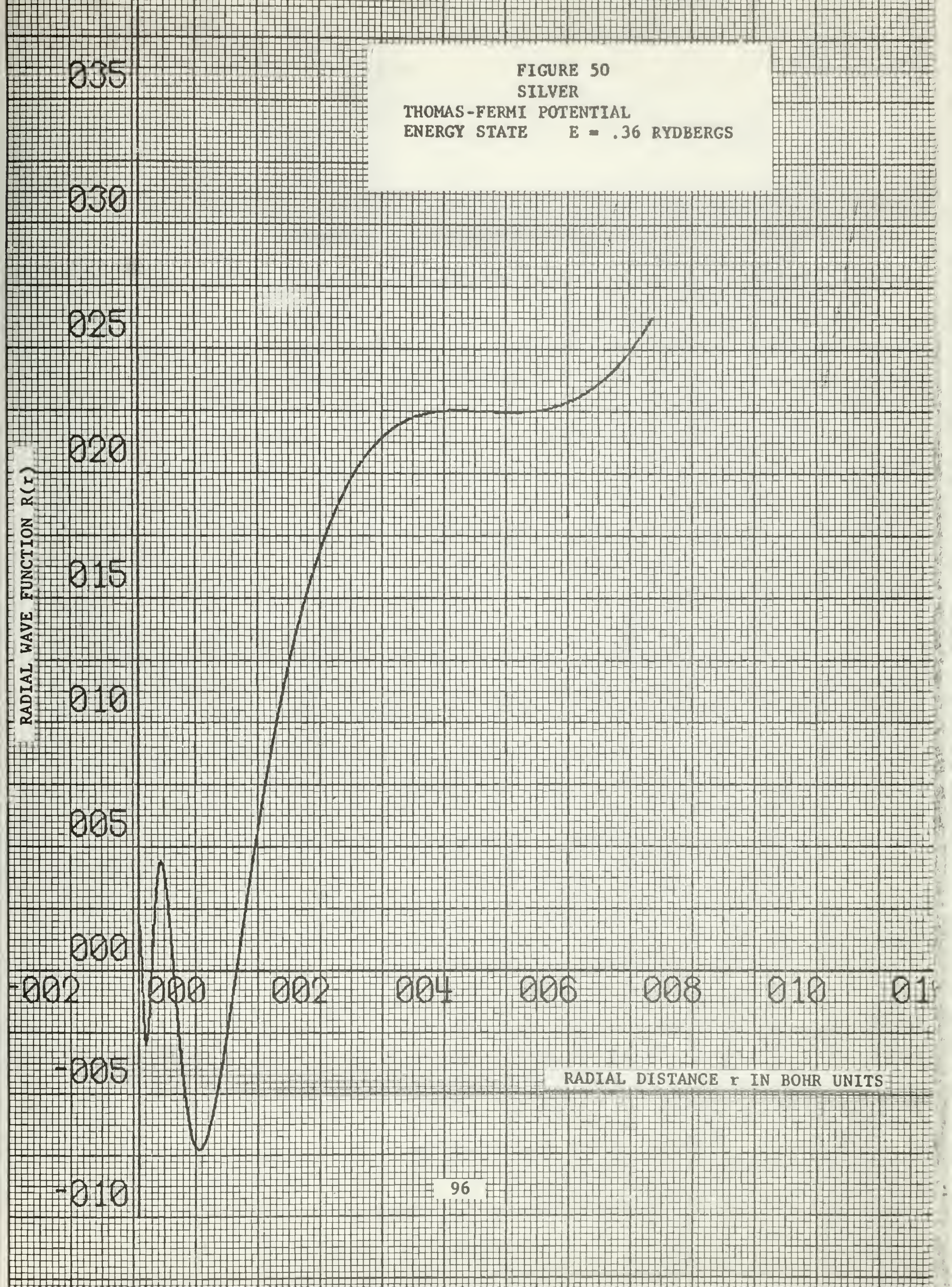


FIGURE 50
SILVER
THOMAS-FERMI POTENTIAL
ENERGY STATE E = .36 RYDBERGS

[illegible]
[illegible]
[illegible]
[illegible]

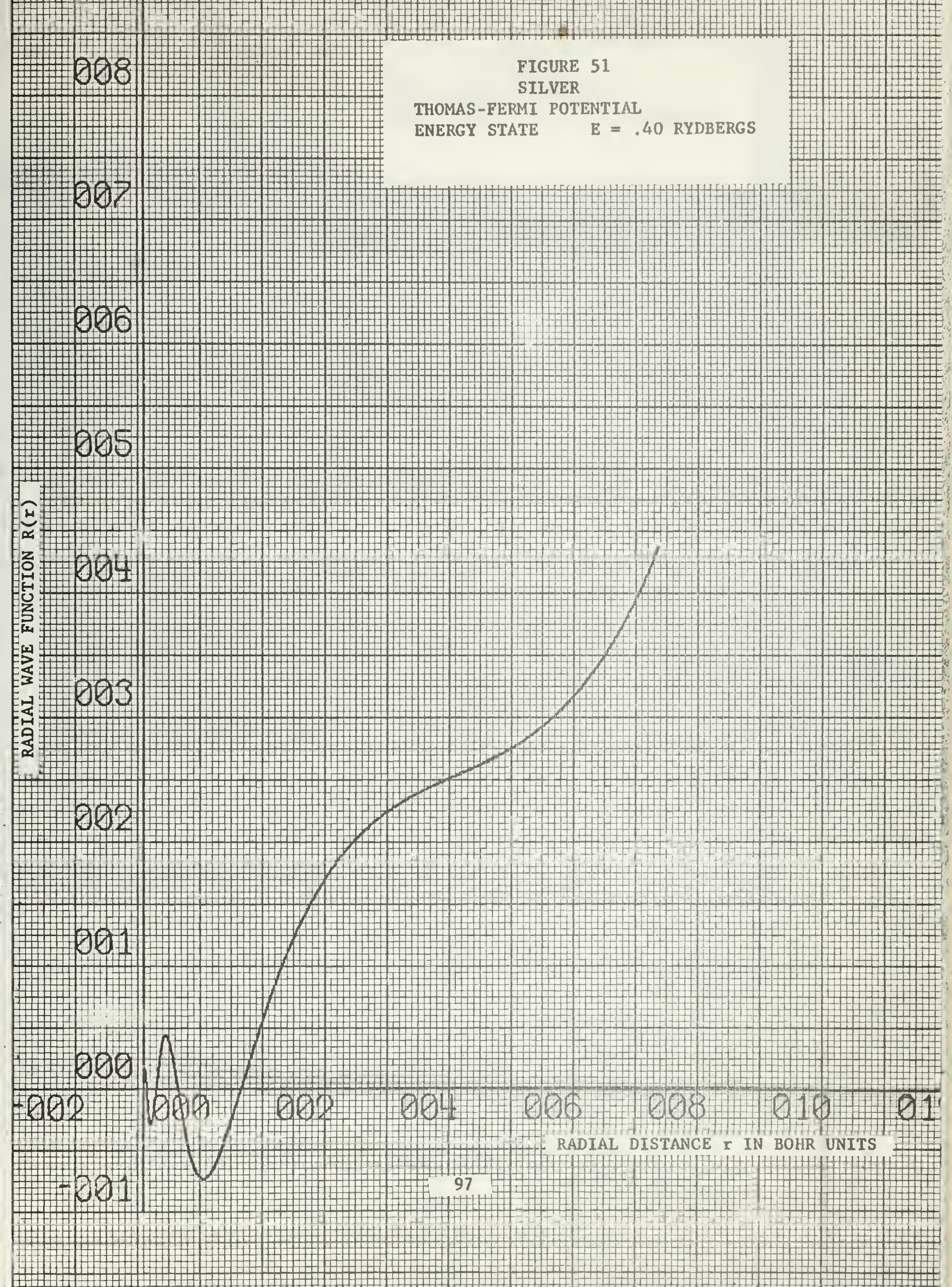


FIGURE 51
SILVER
THOMAS-FERMI POTENTIAL
ENERGY STATE E = .40 RYDBERGS

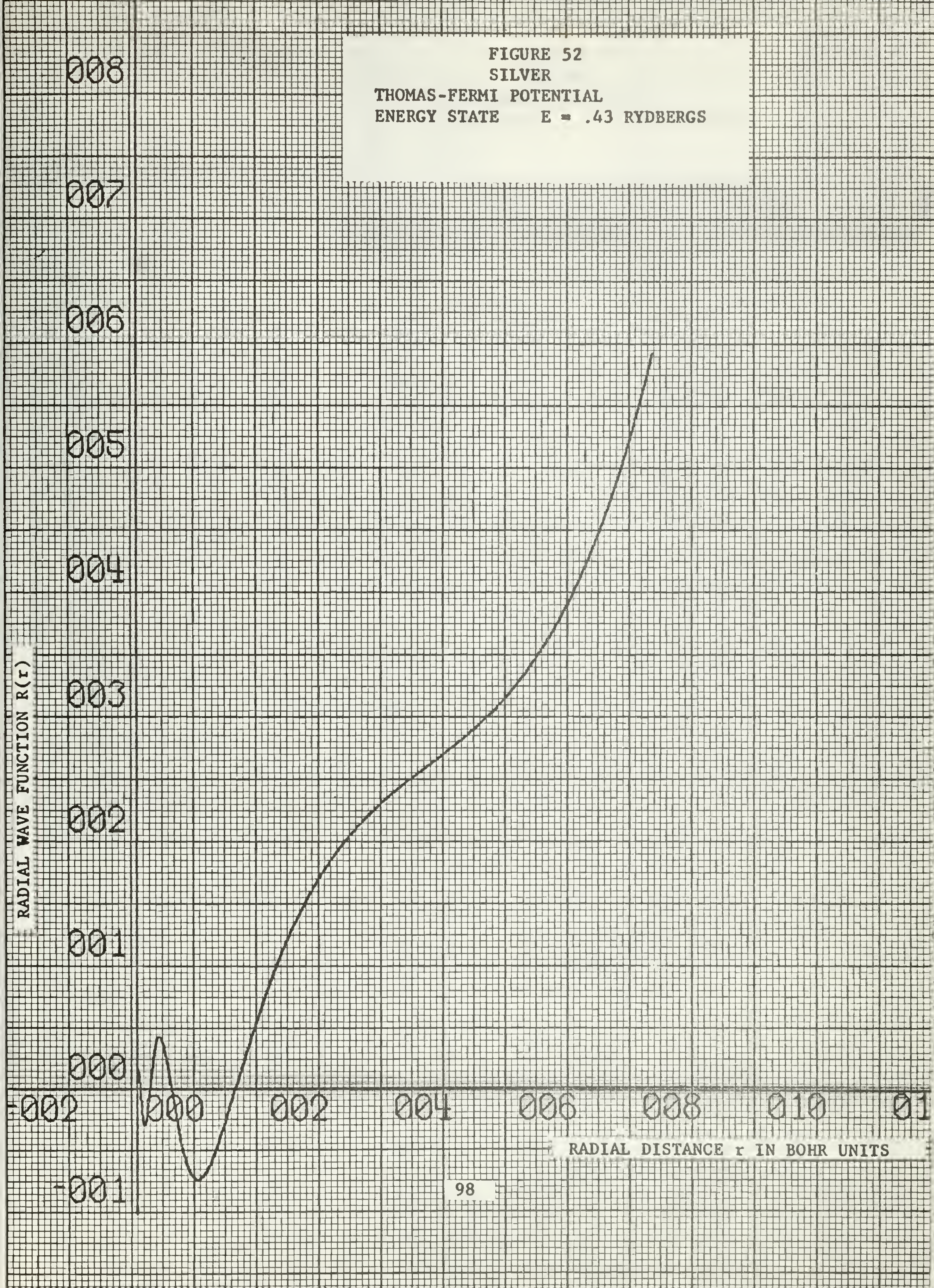


FIGURE 52
SILVER
THOMAS-FERMI POTENTIAL
ENERGY STATE E = .43 RYDBERGS

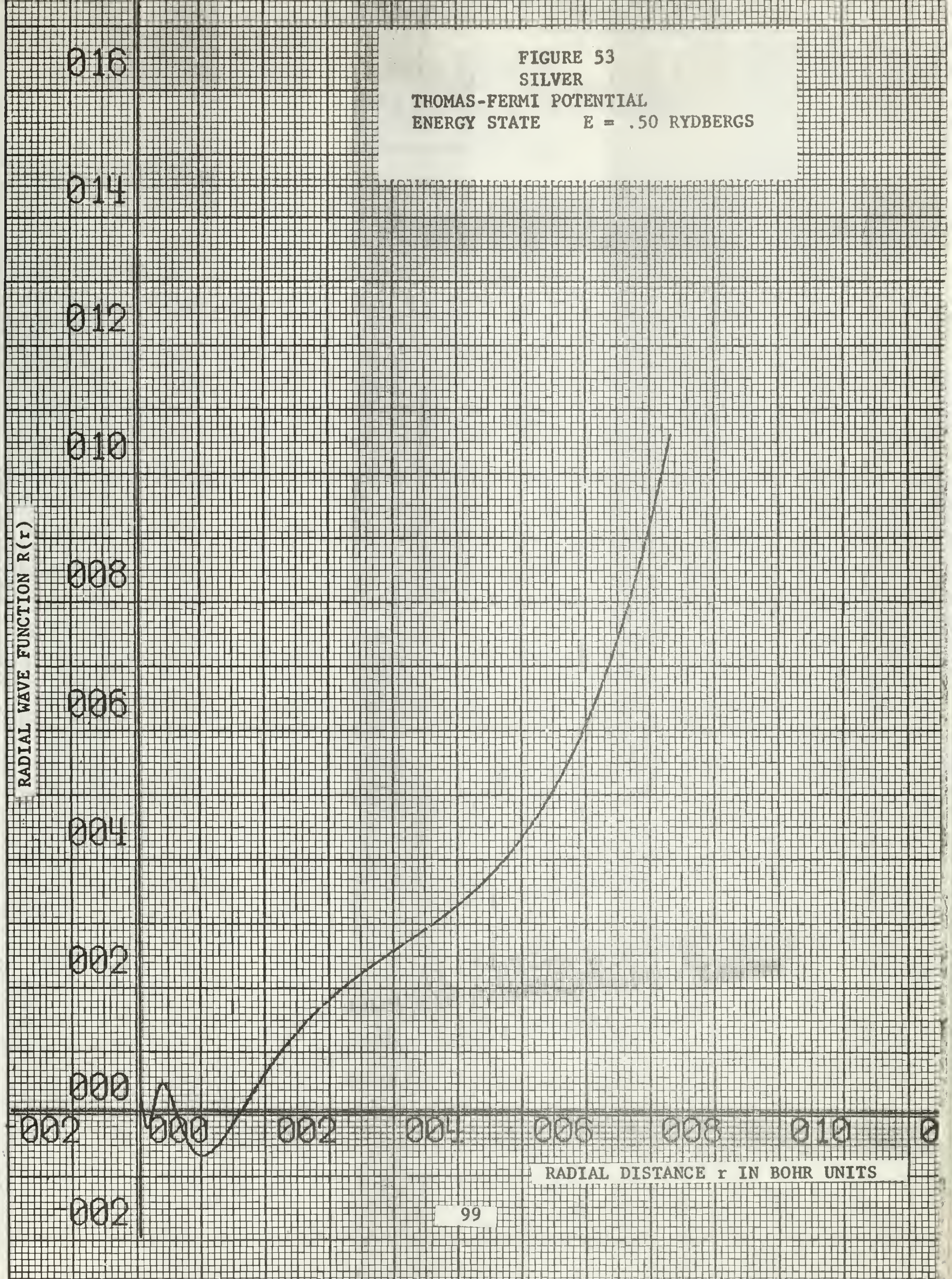


FIGURE 53
SILVER
THOMAS-FERMI POTENTIAL
ENERGY STATE E = .50 RYDBERGS

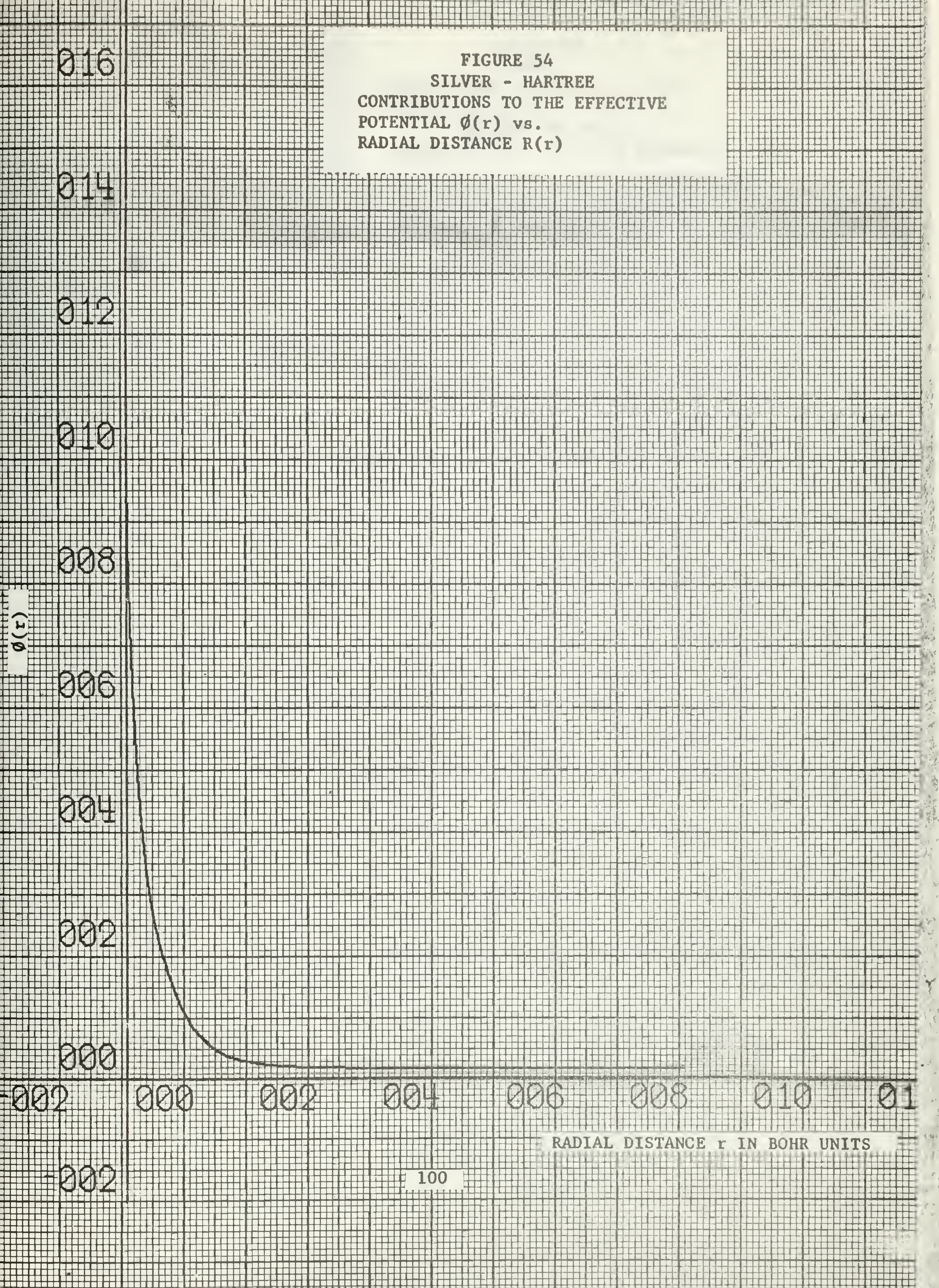
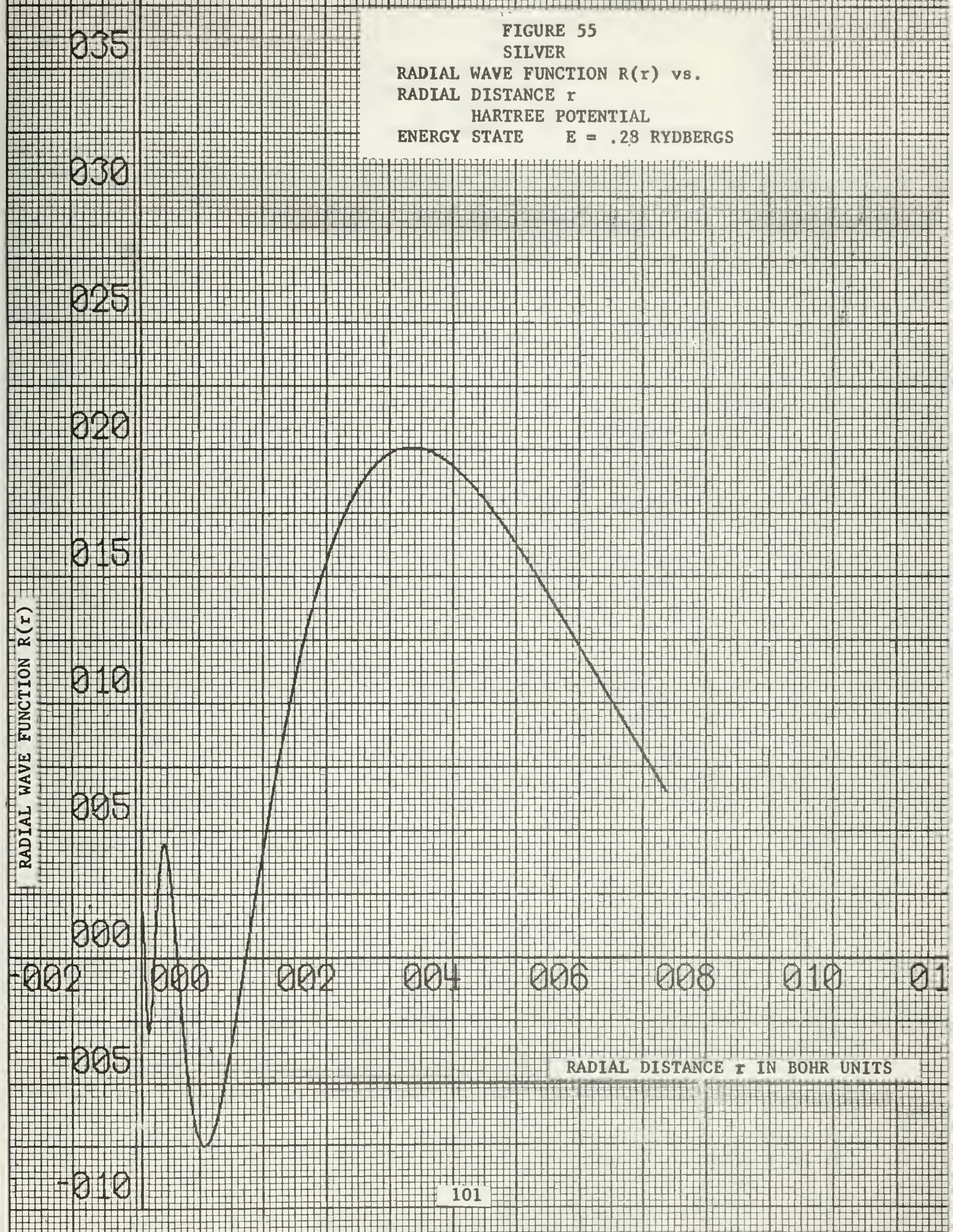


FIGURE 54
SILVER - HARTREE
CONTRIBUTIONS TO THE EFFECTIVE
POTENTIAL Ø(r) vs.
RADIAL DISTANCE R(r)

FIGURE 55
SILVER
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
HARTREE POTENTIAL
ENERGY STATE E = .28 RYDBERGS



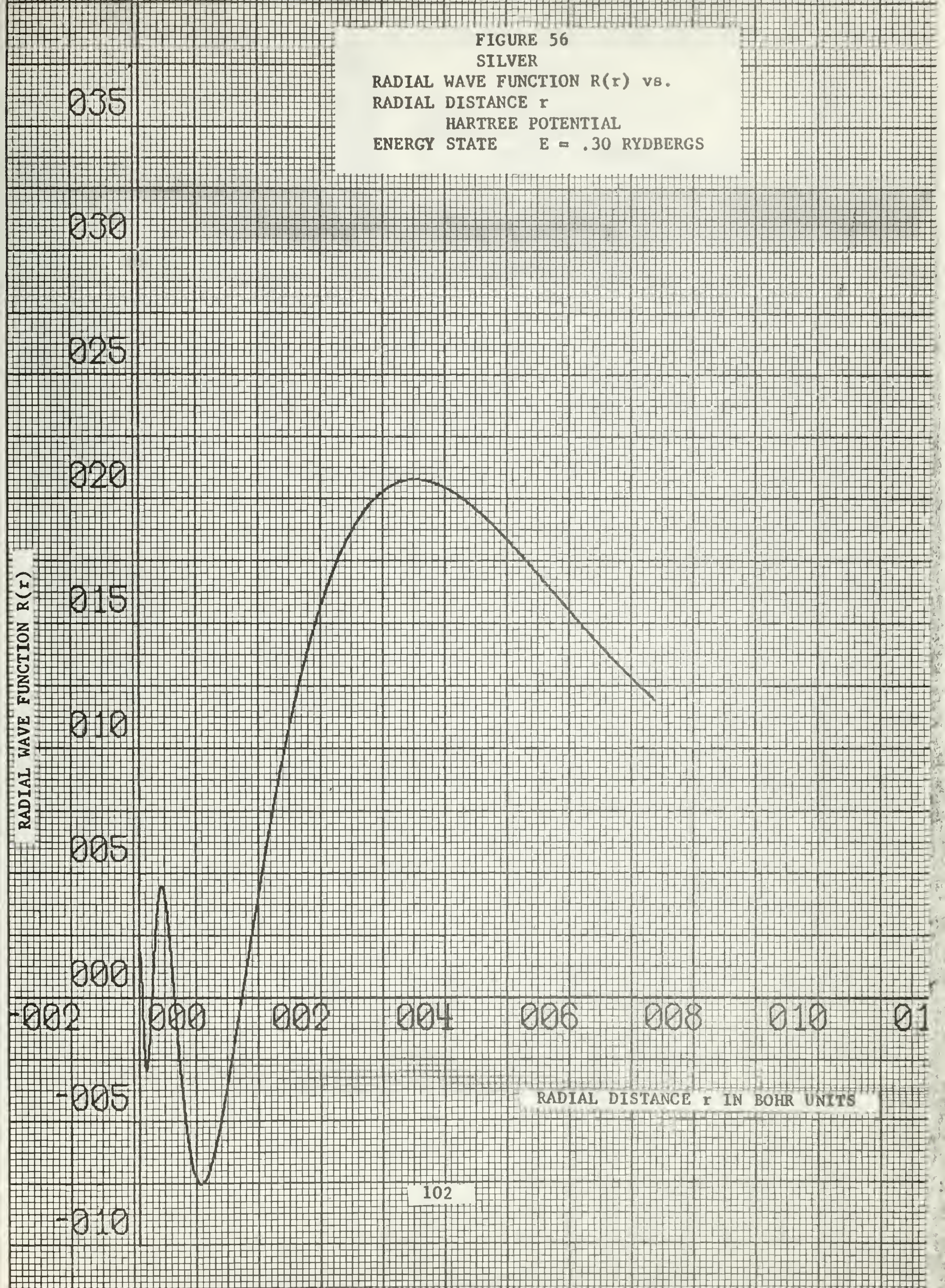


FIGURE 56
SILVER
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
HARTREE POTENTIAL
ENERGY STATE E = .30 RYDBERGS

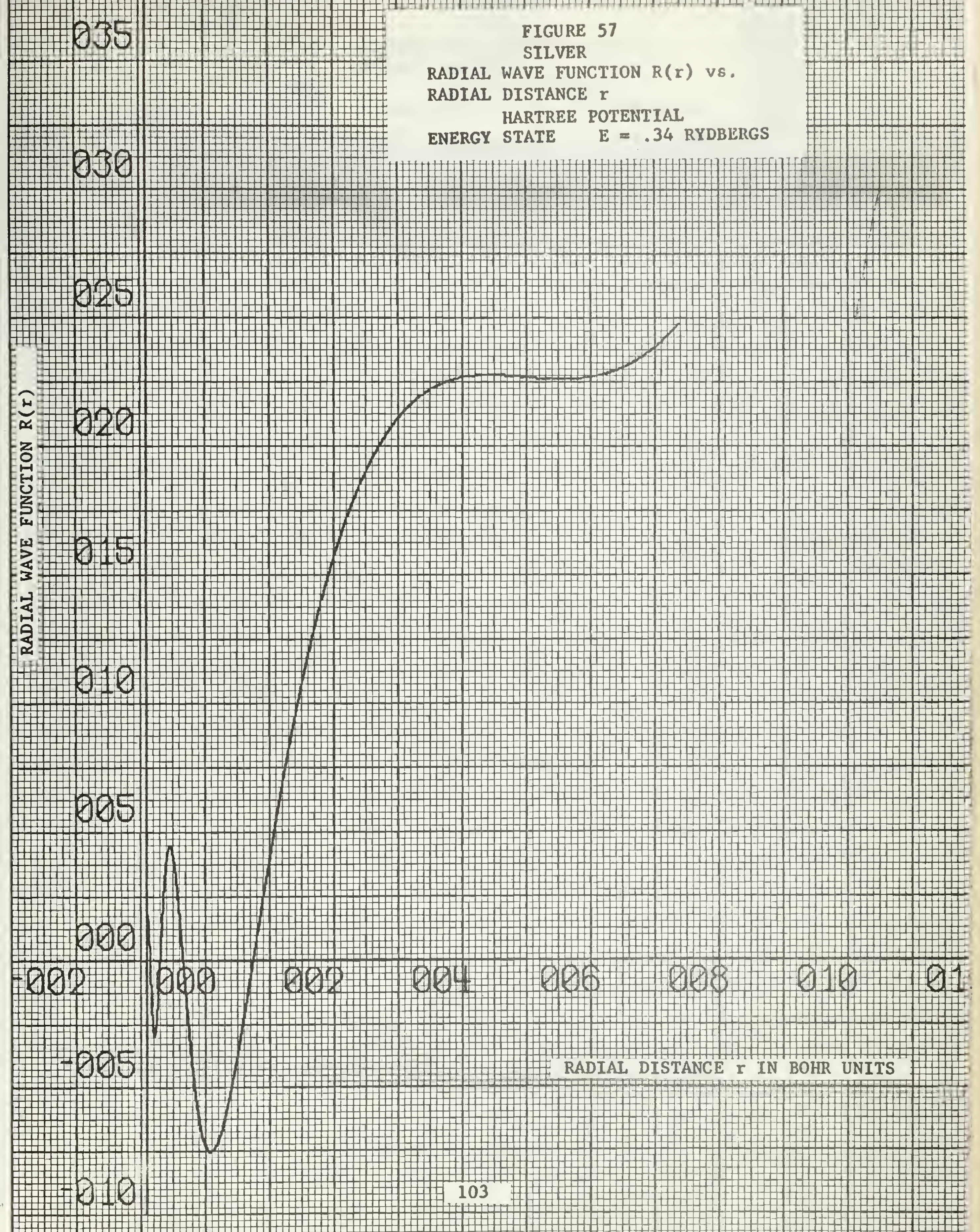


FIGURE 57
SILVER
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
HARTREE POTENTIAL
ENERGY STATE E = .34 RYDBERGS

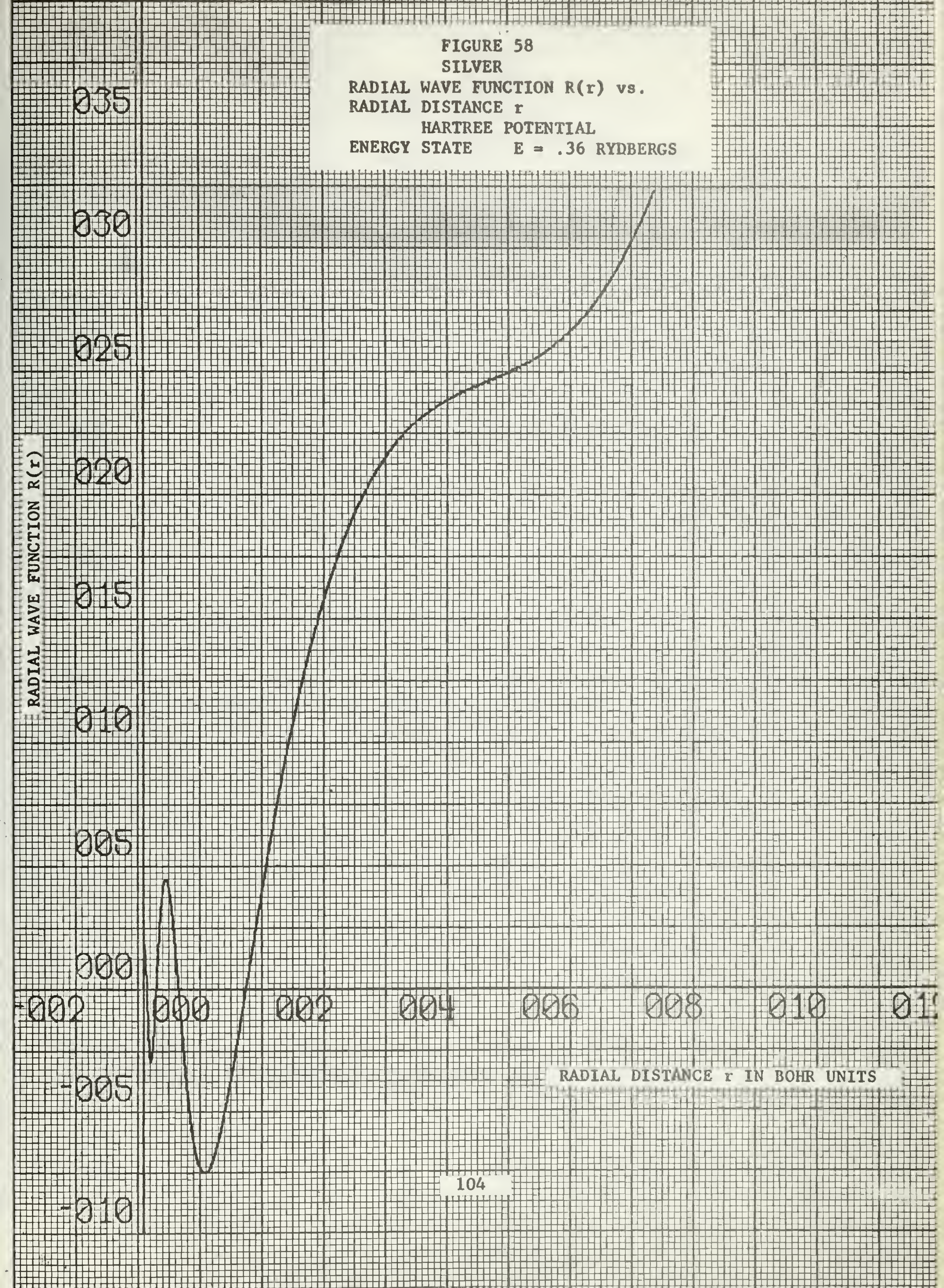
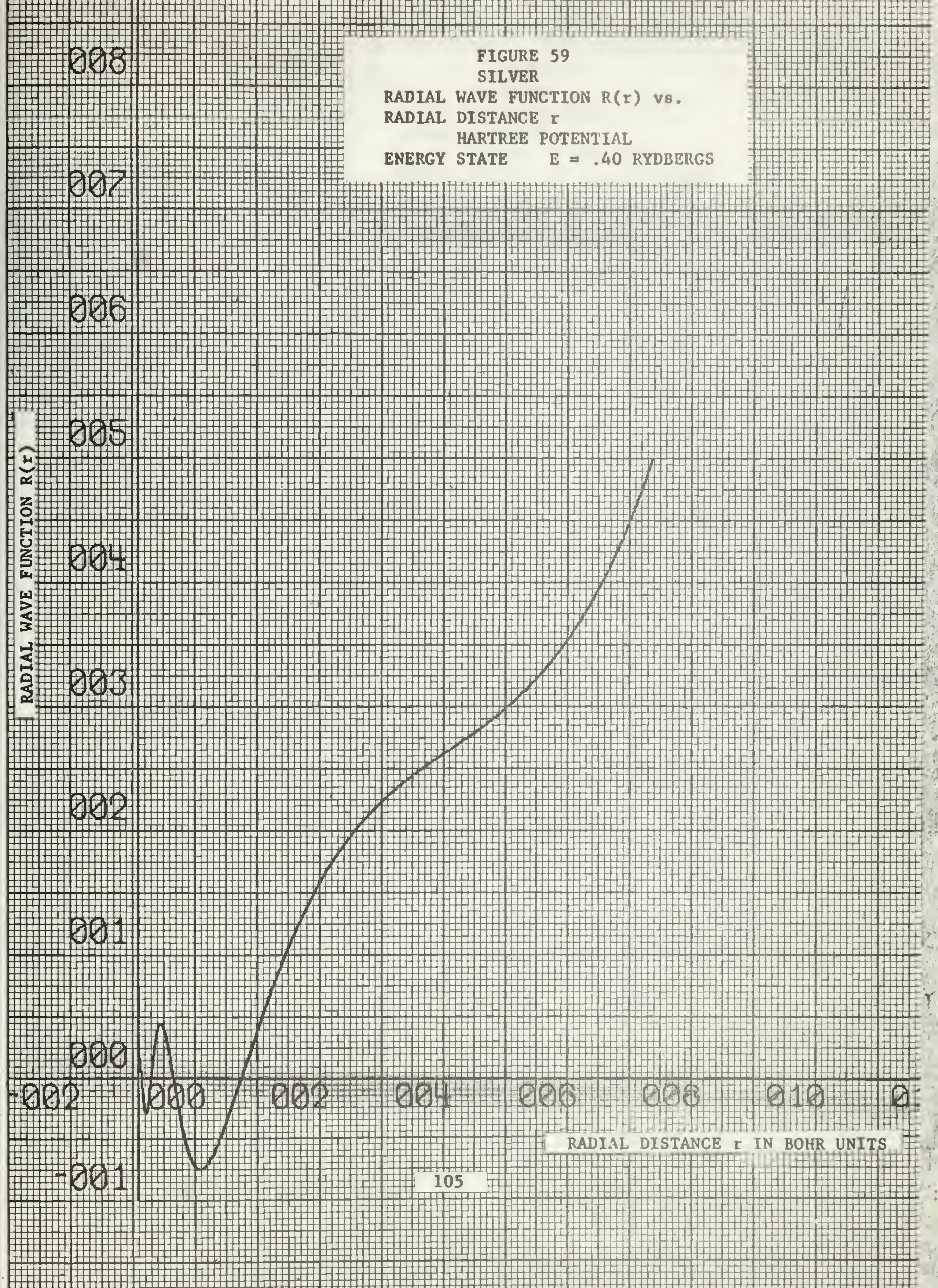


FIGURE 58
SILVER
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
HARTREE POTENTIAL
ENERGY STATE E = .36 RYDBERGS

FIGURE 59
SILVER
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
HARTREE POTENTIAL
ENERGY STATE E = .40 RYDBERGS



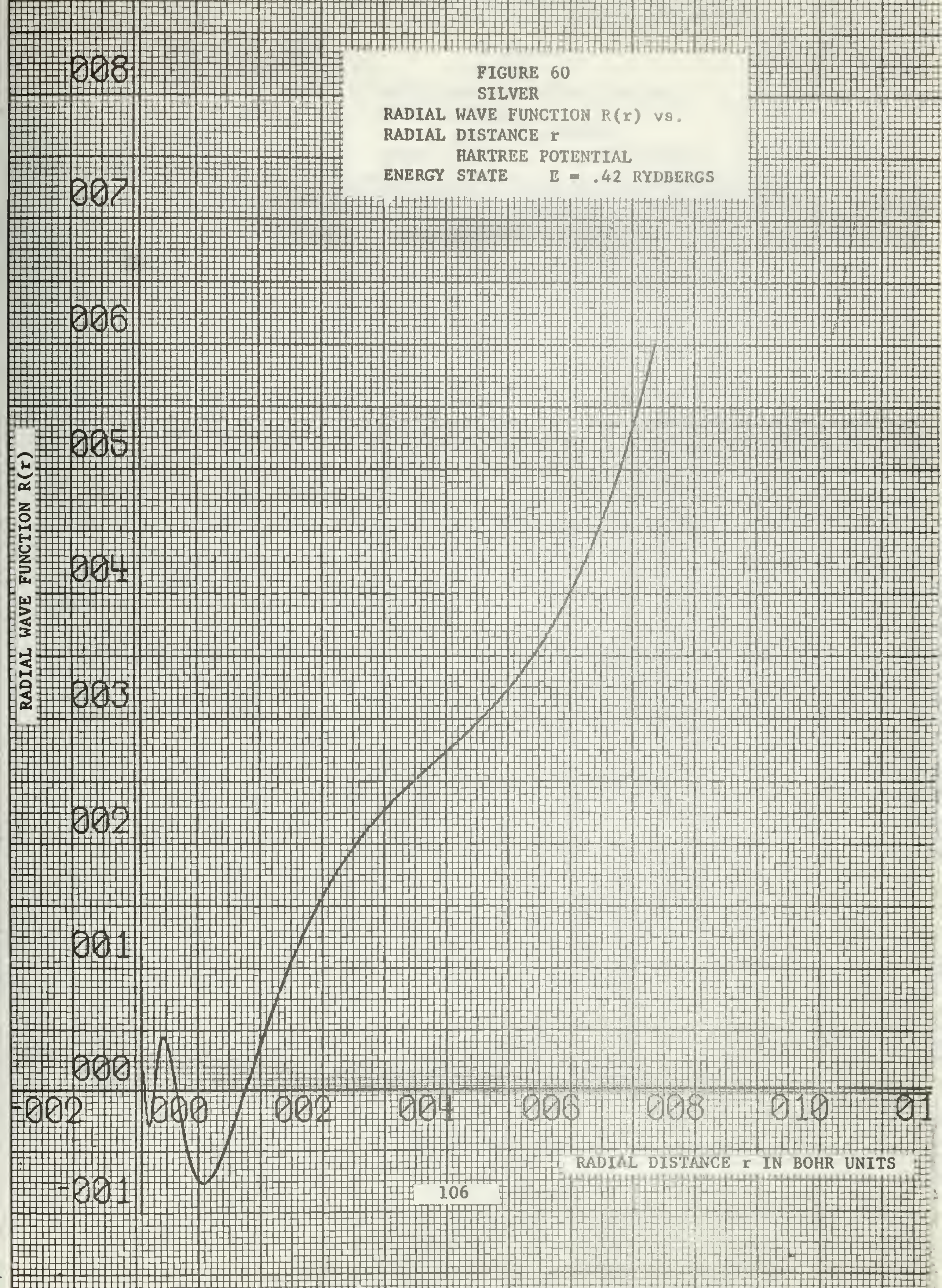


FIGURE 60
SILVER
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
HARTREE POTENTIAL
ENERGY STATE E = .42 RYDBERGS

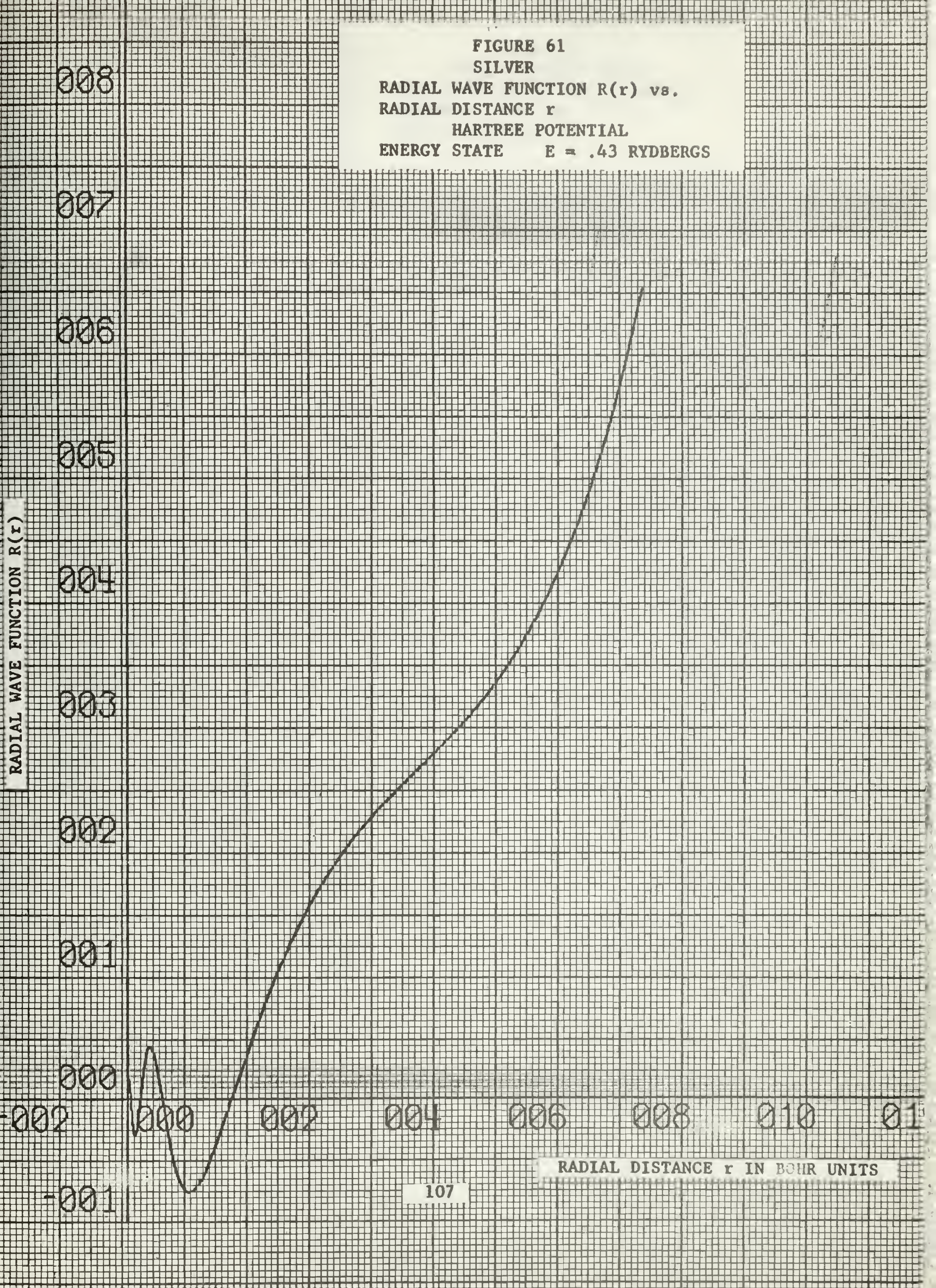


FIGURE 61
SILVER
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
HARTREE POTENTIAL
ENERGY STATE E = .43 RYDBERGS

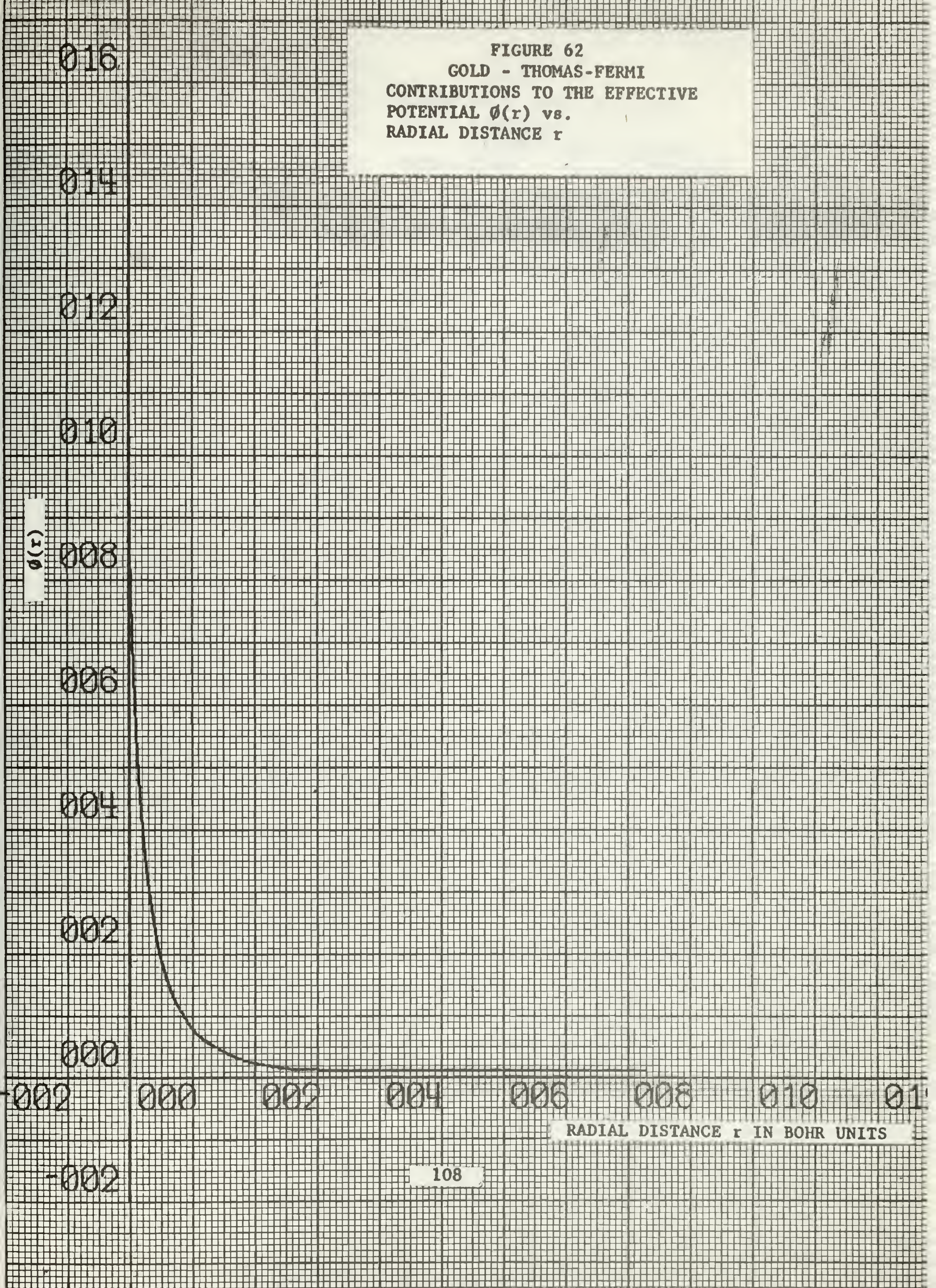


FIGURE 62
GOLD - THOMAS-FERMI
CONTRIBUTIONS TO THE EFFECTIVE
POTENTIAL $\phi(r)$ vs.
RADIAL DISTANCE r

[illegible]

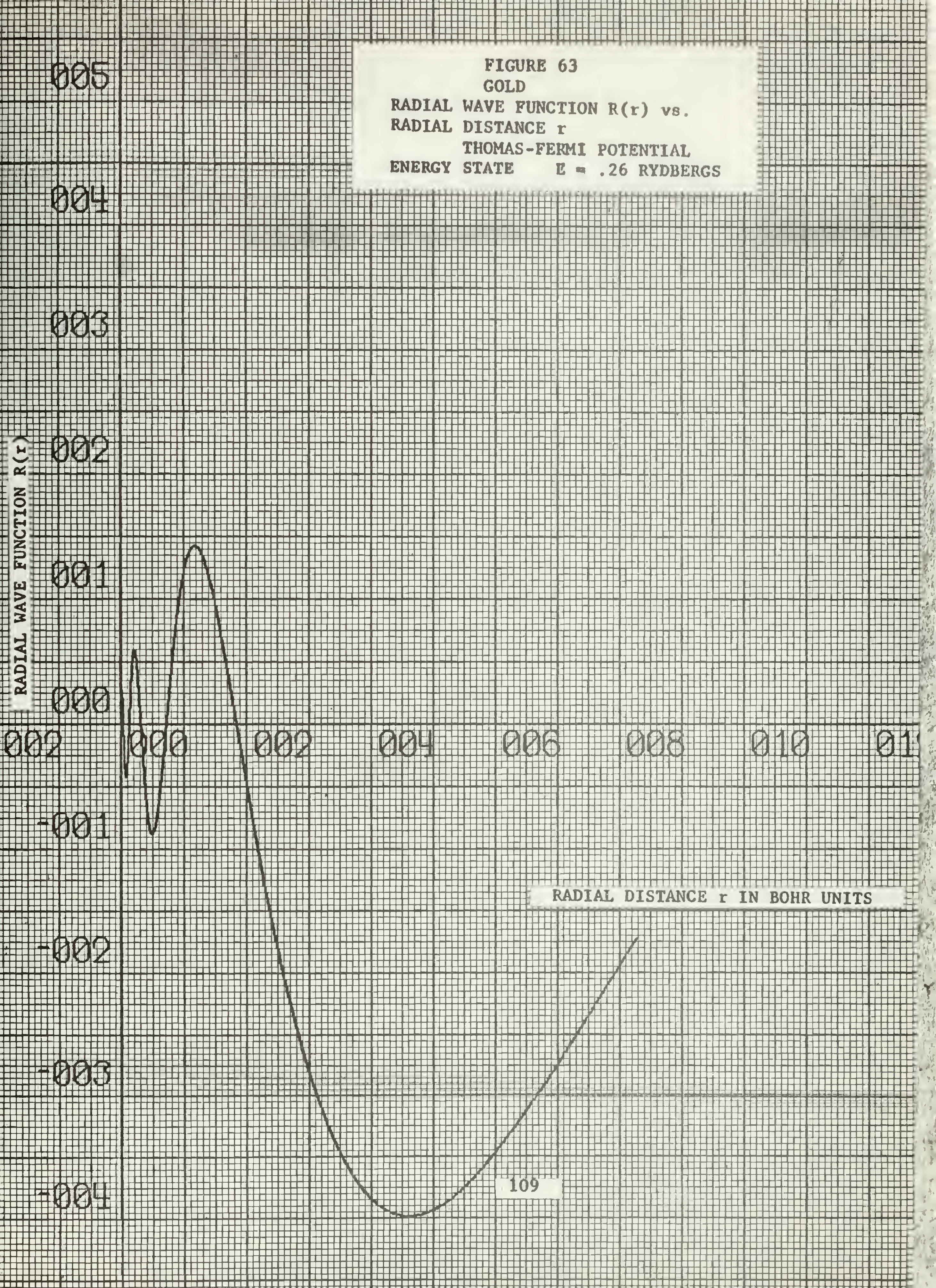


FIGURE 63
GOLD
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
THOMAS-FERMI POTENTIAL
ENERGY STATE E = .26 RYDBERGS

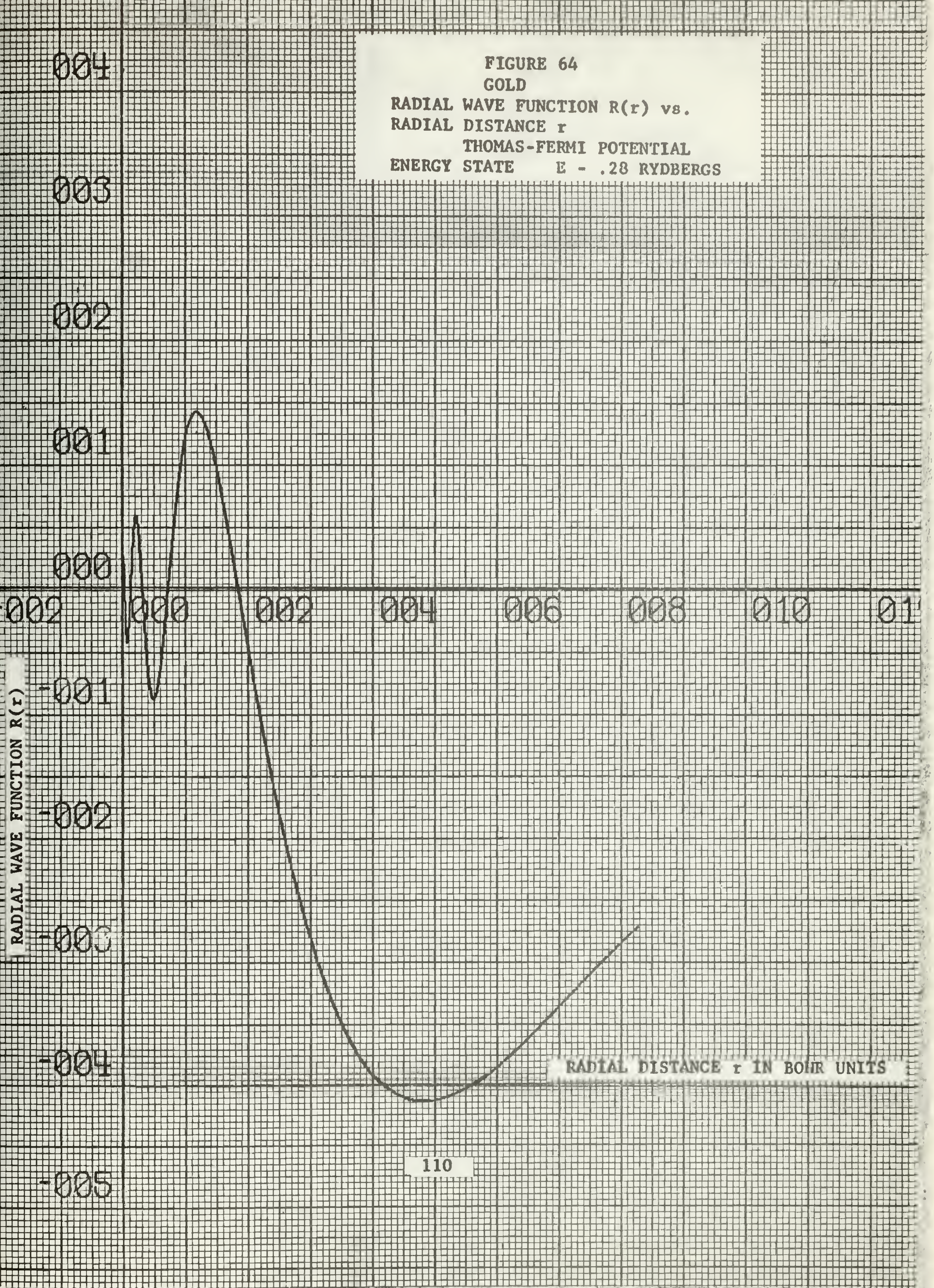


FIGURE 64
GOLD
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
THOMAS-FERMI POTENTIAL
ENERGY STATE E - .28 RYDBERGS

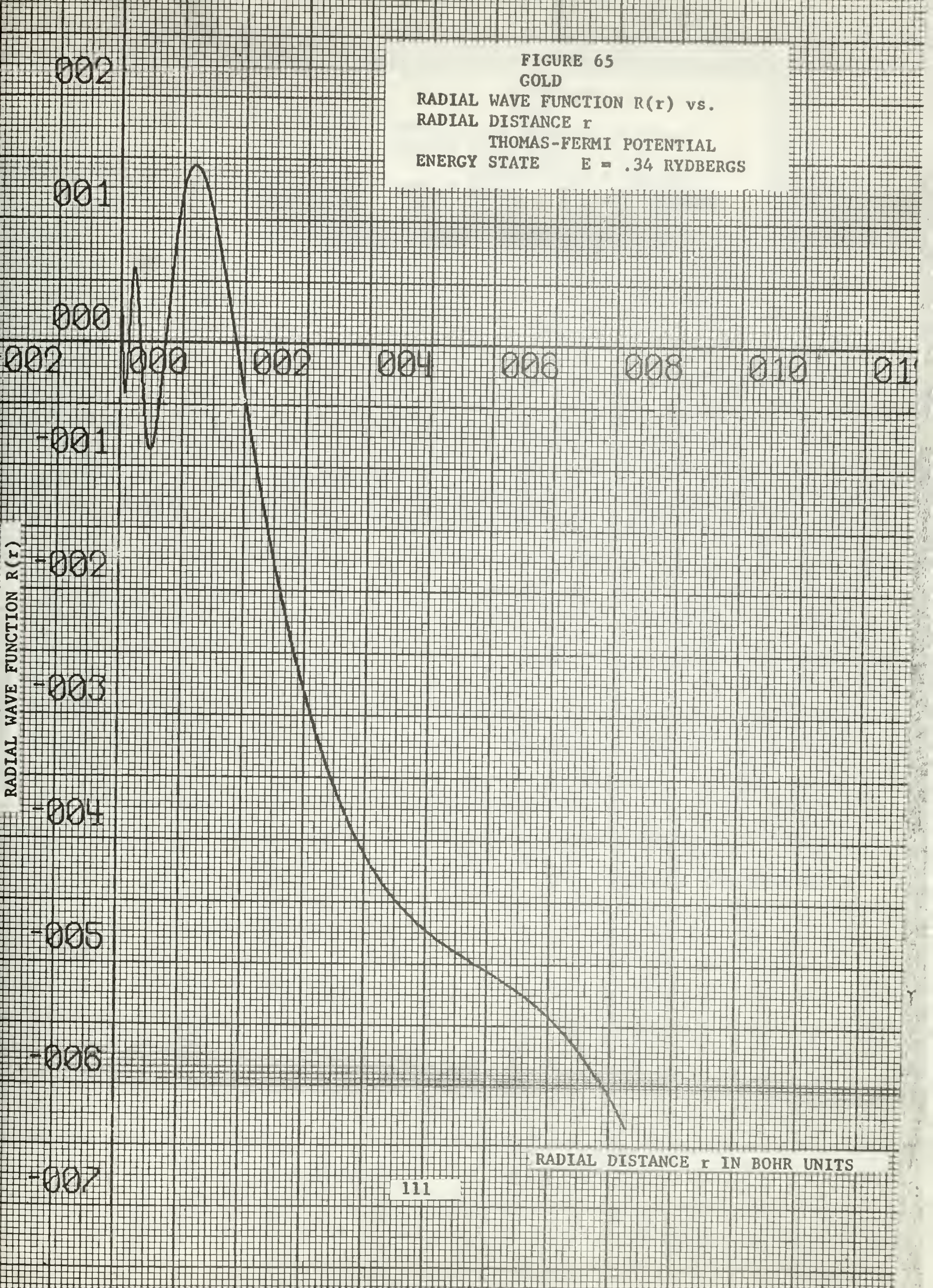


FIGURE 65
GOLD
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
THOMAS-FERMI POTENTIAL
ENERGY STATE E = .34 RYDBERGS

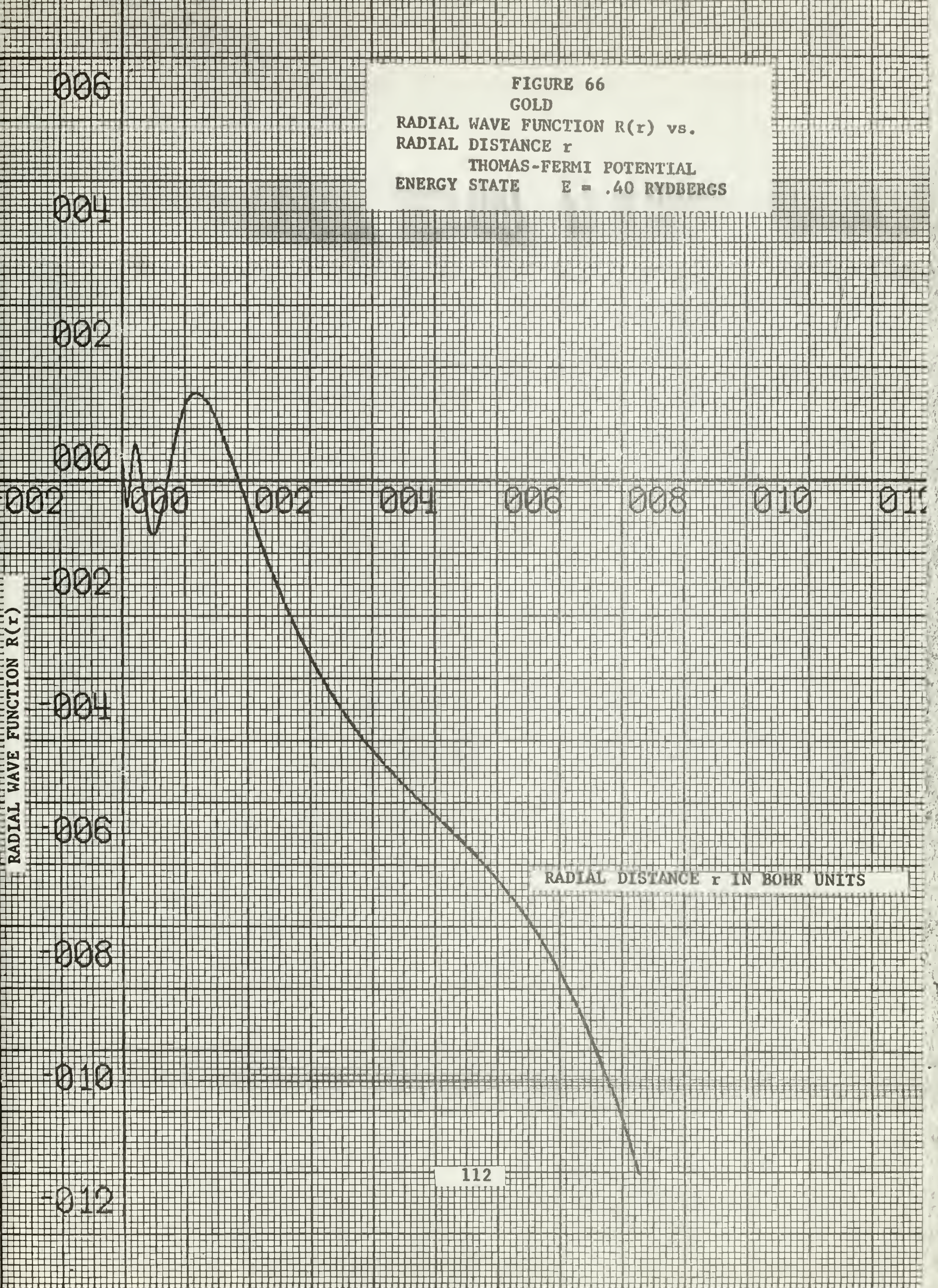


FIGURE 66
GOLD
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
THOMAS-FERMI POTENTIAL
ENERGY STATE E = .40 RYDBERGS

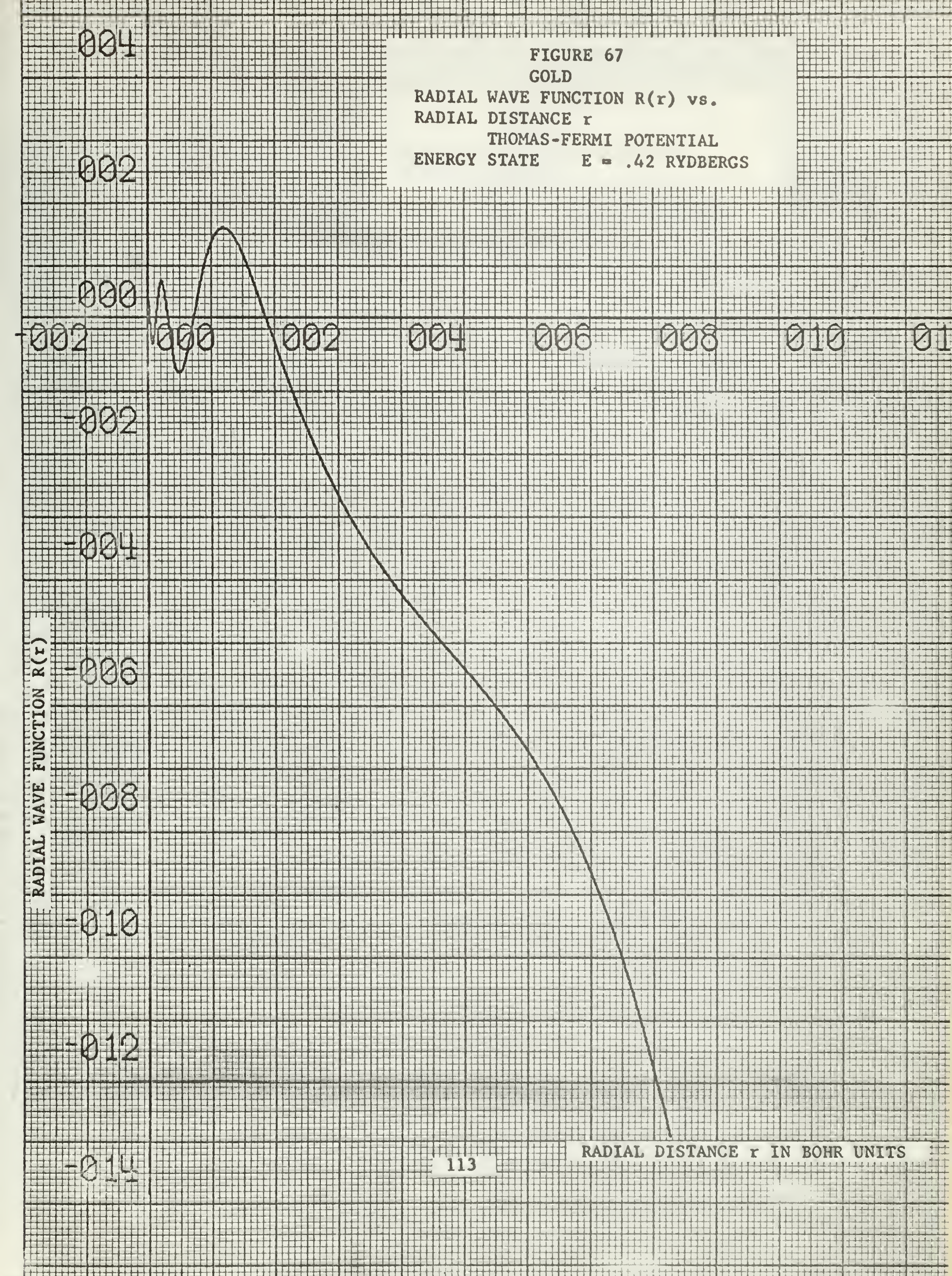


FIGURE 67
GOLD
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
THOMAS-FERMI POTENTIAL
ENERGY STATE E = .42 RYDBERGS

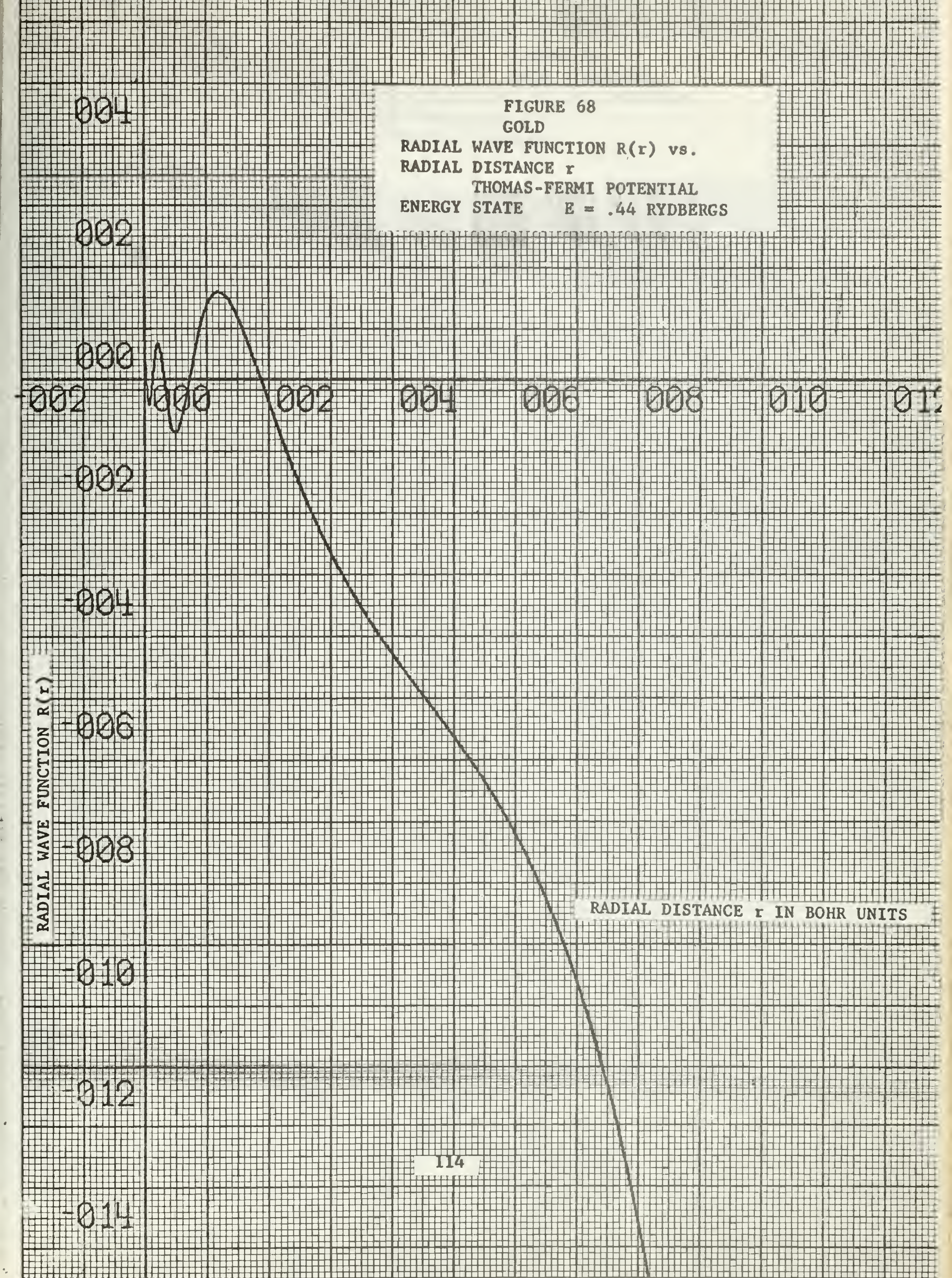


FIGURE 68
GOLD
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
THOMAS-FERMI POTENTIAL
ENERGY STATE E = .44 RYDBERGS

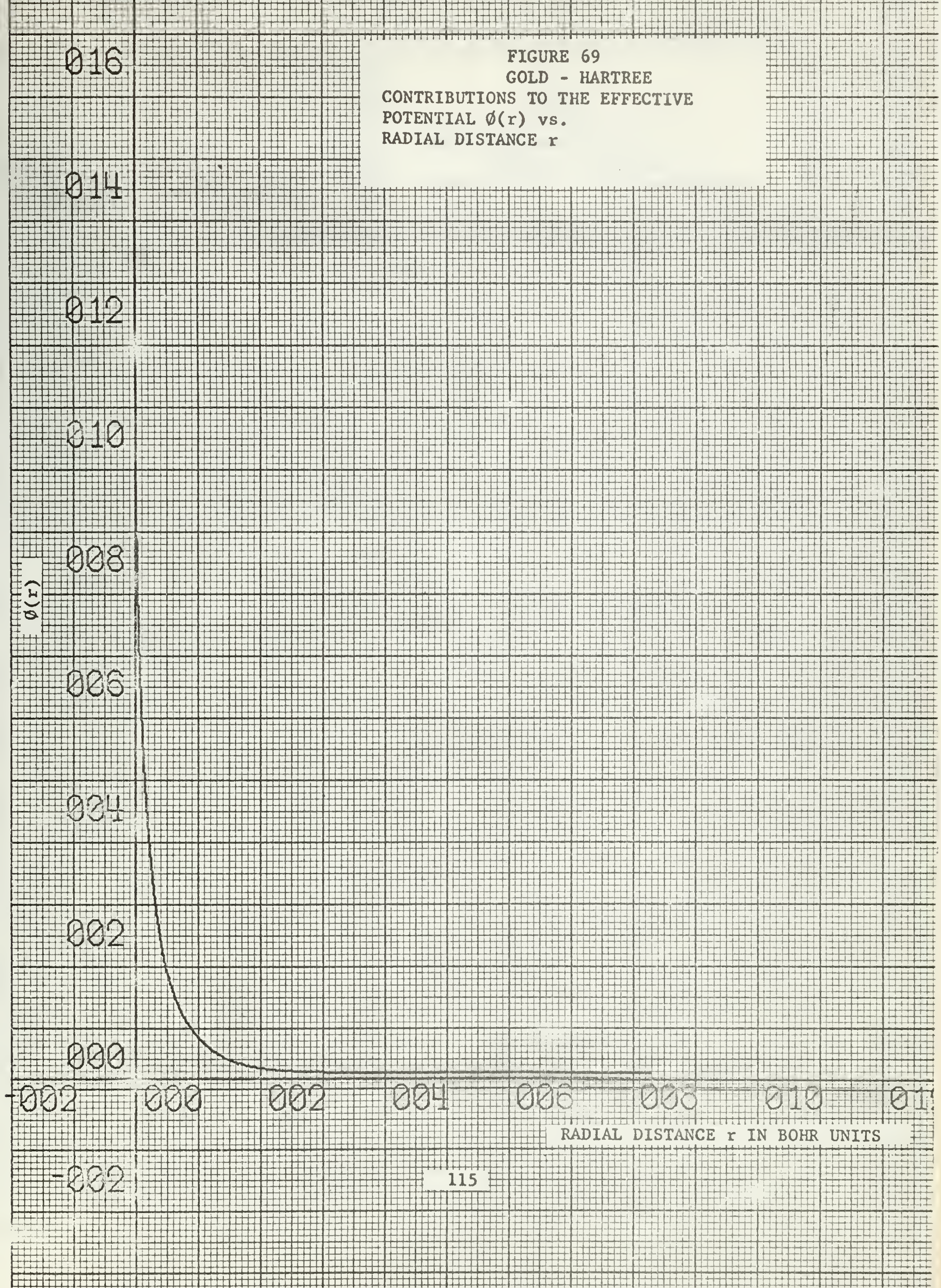


FIGURE 69
GOLD - HARTREE
CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL Ø(r) vs. RADIAL DISTANCE r

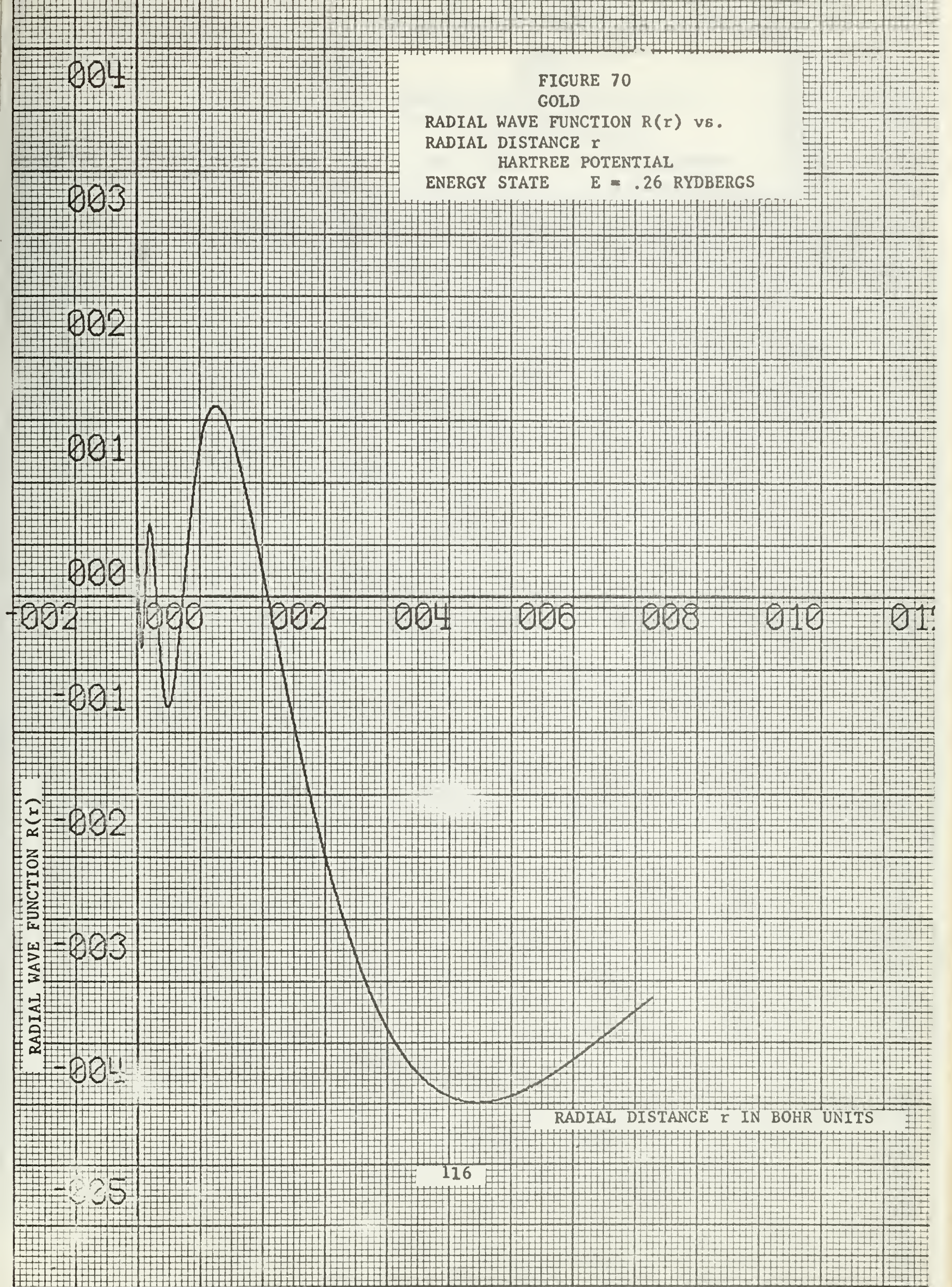


FIGURE 70
GOLD
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
HARTREE POTENTIAL
ENERGY STATE E = .26 RYDBERGS

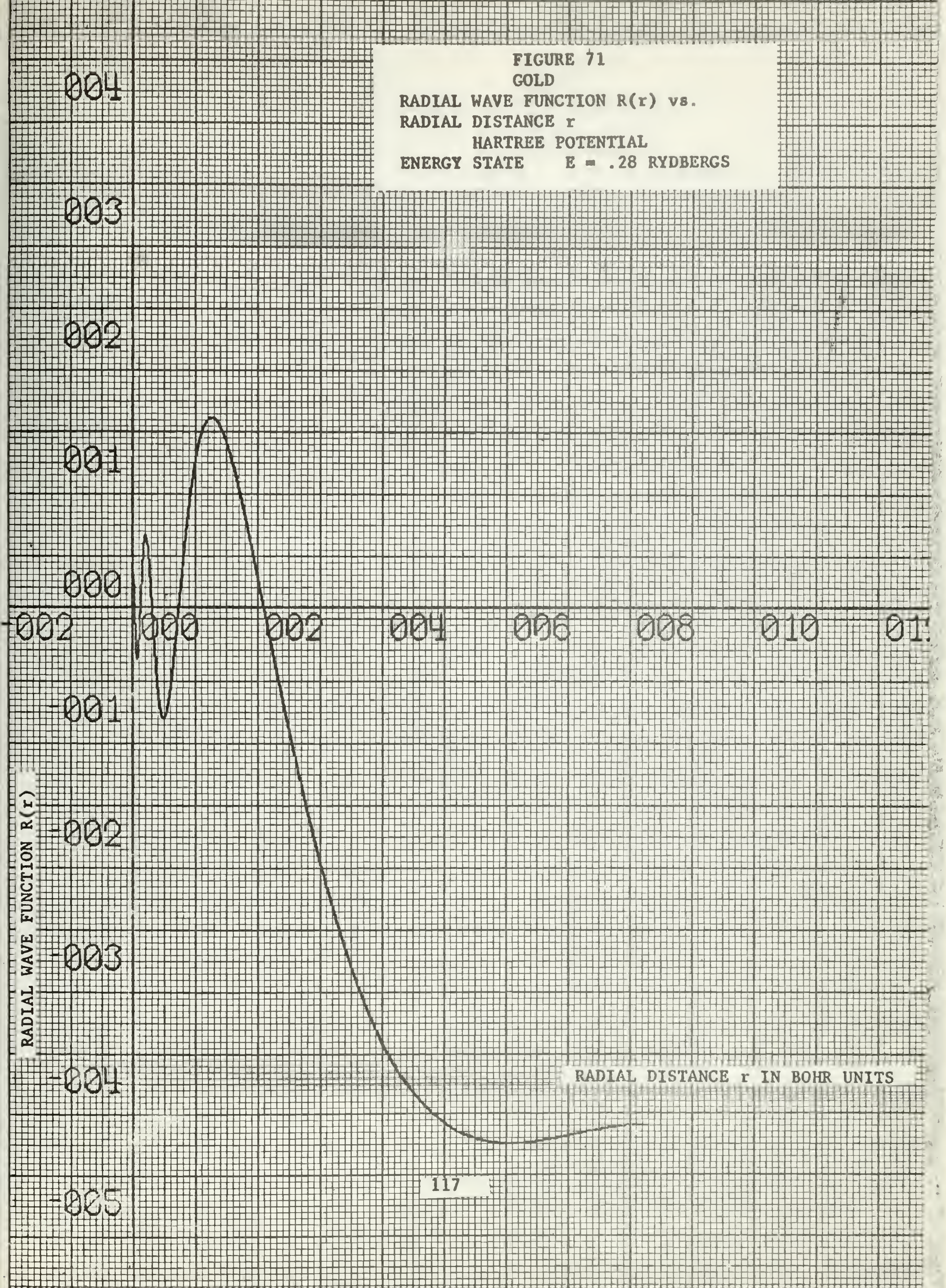


FIGURE 71
GOLD
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
HARTREE POTENTIAL
ENERGY STATE E = .28 RYDBERGS

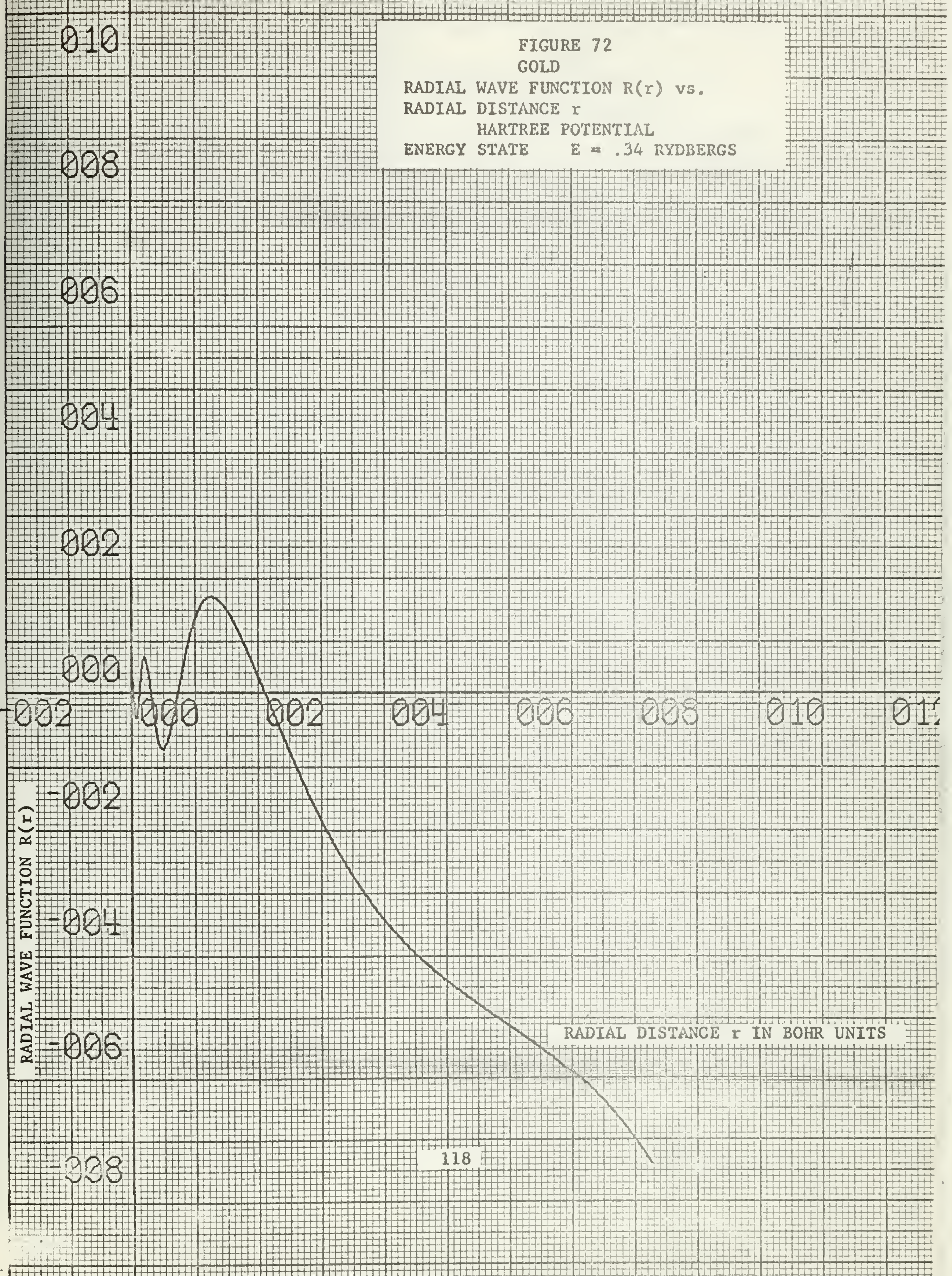


FIGURE 72
GOLD
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
HARTREE POTENTIAL
ENERGY STATE E = .34 RYDBERGS

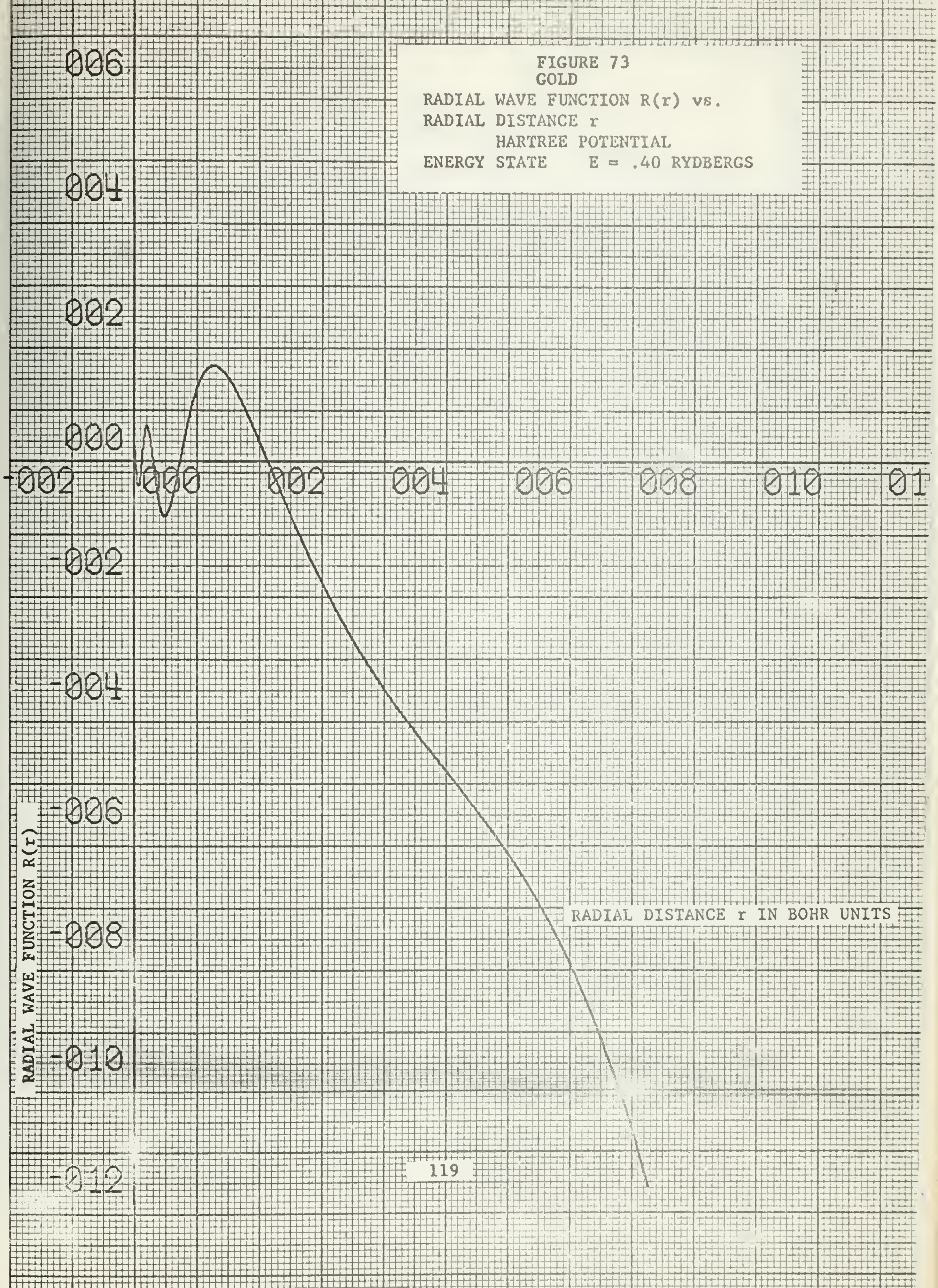


FIGURE 73
GOLD
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
HARTREE POTENTIAL
ENERGY STATE E = .40 RYDBERGS

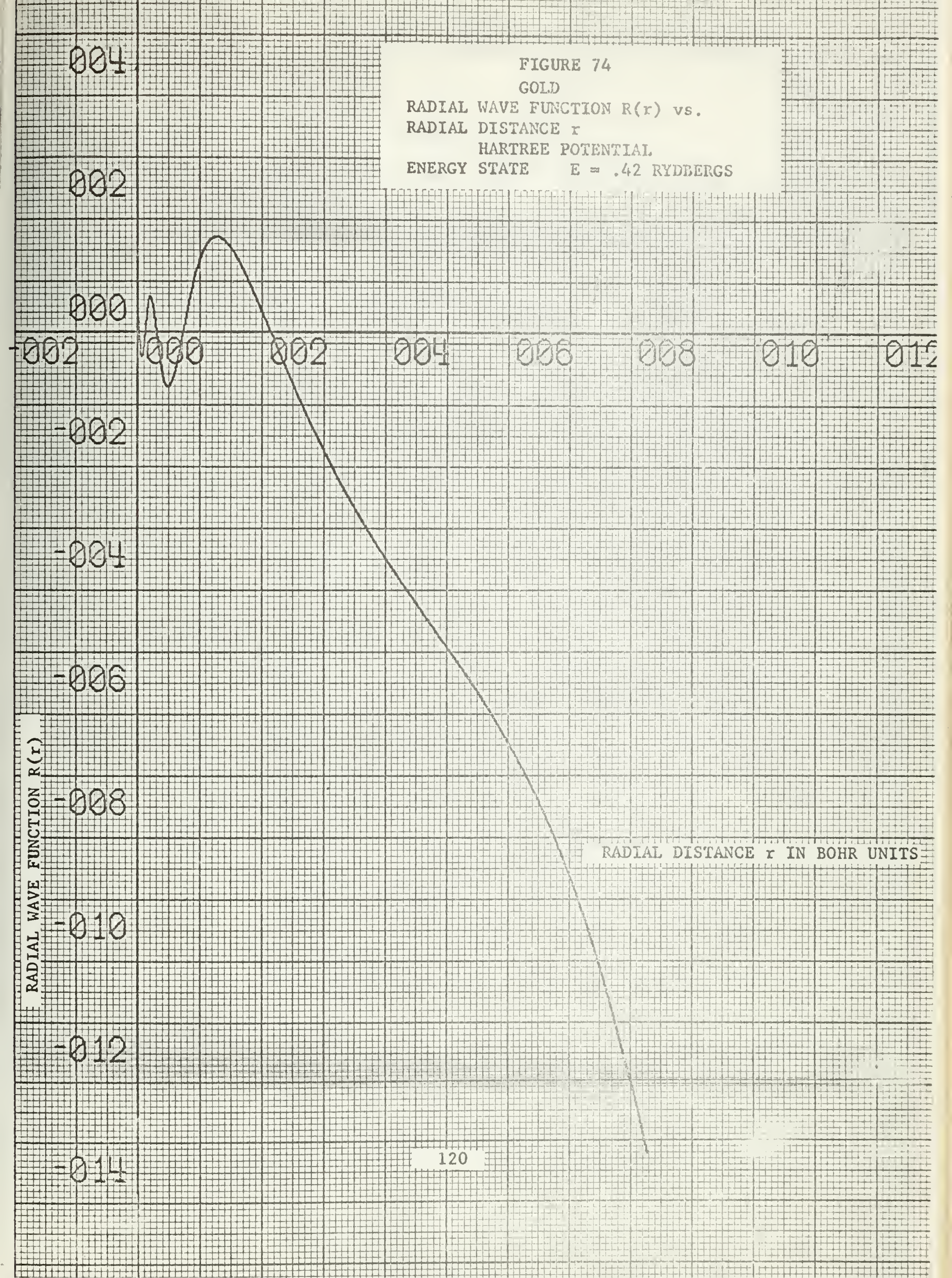


FIGURE 74
GOLD
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
HARTREE POTENTIAL
ENERGY STATE E = .42 RYDBERGS

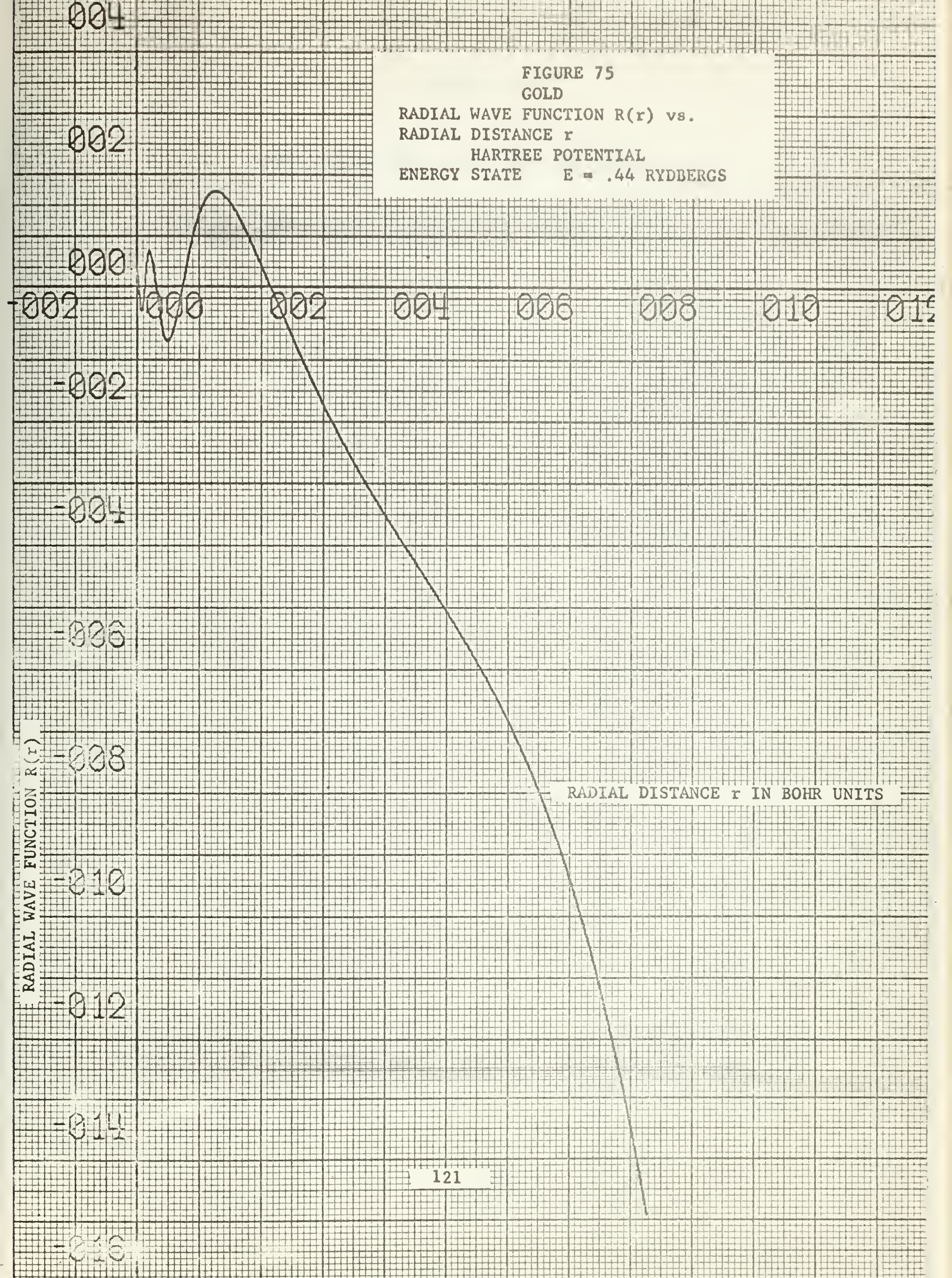


FIGURE 75
GOLD
RADIAL WAVE FUNCTION R(r) vs.
RADIAL DISTANCE r
HARTREE POTENTIAL
ENERGY STATE E = .44 RYDBERGS

APPENDIX III

TABULATED VALUES OF THE WAVE FUNCTIONS OF GOLD

TABLE V

GCLC

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL AND THE RADIAL WAVE FUNCTION. IONIZATION ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100 BOHR UNITS.

R	PHI(R)	R(R)
1	8.90109944E-01	7.63658744E-03
2	8.46086760E-01	2.30568699E-02
3	8.13447670E-01	2.97255693E-02
4	7.86723391E-01	1.86613459E-02
5	7.63776204E-01	1.79924425E-03
6	7.43504227E-01	-1.54969999E-02
7	7.25259941E-01	-2.97601097E-02
8	7.08587379E-01	-3.91534965E-02
9	6.93217220E-01	-4.30701115E-02
10	6.78922125E-01	-4.17480428E-02
11	6.65538998E-01	-3.59504547E-02
12	6.52940877E-01	-2.67155555E-02
13	6.41026945E-01	-1.51914269E-02
14	6.29715610E-01	-2.48175468E-03
15	6.18939770E-01	1.04041254E-02
16	6.08643480E-01	2.26124015E-02
17	5.98779544E-01	3.34630092E-02
18	5.89307727E-01	4.24537594E-02
19	5.80197422E-01	4.92511949E-02
20	5.71406617E-01	5.36756552E-02
21	5.62921098E-01	5.56807111E-02
22	5.54713319E-01	5.53712239E-02
23	5.46764399E-01	5.27911068E-02
24	5.39054720E-01	4.82520287E-02
25	5.31562598E-01	4.20138074E-02
26	5.24291507E-01	3.43669247E-02
27	5.17210366E-01	2.56273733E-02
28	5.10313328E-01	1.61133908E-02
29	5.03589653E-01	6.13744016E-03
30	4.97029527E-01	-4.00698049E-03
31	4.90624167E-01	-1.40467797E-02
32	4.84365225E-01	-2.37362406E-02
33	4.78245549E-01	-3.28596569E-02
34	4.72257724E-01	-4.10328278E-02
35	4.66395072E-01	-4.87039461E-02
36	4.60652594E-01	-5.51526774E-02
37	4.55024426E-01	-6.04901310E-02
38	4.49305492E-01	-6.46562433E-02
39	4.44091074E-01	-6.76192387E-02
40	4.38776722E-01	-6.93681919E-02
41	4.33558502E-01	-6.99004976E-02
42	4.28432409E-01	-6.97092377E-02
43	4.23591009E-01	-6.79855217E-02
44	4.18442637E-01	-6.48148586E-02
45	4.13572468E-01	-6.10746109E-02
46	4.08791342E-01	-5.64515671E-02
47	4.04066537E-01	-5.10396606E-02
48	3.99425449E-01	-4.49378554E-02
49	3.94955538E-01	-3.82482111E-02
50	3.90354479E-01	-3.10741351E-02

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL AND THE RADIAL WAVE FUNCTION. IONIZATION ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100 BOHR UNITS.

R	PHI(R)	R(R)
51	3.85920057E-01	-2.35188228E-02
52	3.81550175E-01	-1.56848870E-02
53	3.77242849E-01	-7.66816834E-03
54	3.72996196E-01	4.33276630E-04
55	3.68808431E-01	8.53002185E-03
56	3.64677857E-01	1.65359608E-02
57	3.60602864E-01	2.43748502E-02
58	3.56551917E-01	3.19707203E-02
59	3.52613558E-01	3.92581631E-02
60	3.48696396E-01	4.61775106E-02
61	3.44822106E-01	5.26759160E-02
62	3.41010423E-01	5.87073474E-02
63	3.37230139E-01	6.42325062E-02
64	3.33514103E-01	6.92196808E-02
65	3.29834210E-01	7.36395445E-02
66	3.26192406E-01	7.74749068E-02
67	3.22605683E-01	8.07104831E-02
68	3.19055073E-01	8.33573026E-02
69	3.15545649E-01	8.53519198E-02
70	3.12076523E-01	8.67555079E-02
71	3.08646847E-01	8.75537669E-02
72	3.05255799E-01	8.77564959E-02
73	3.01902593E-01	8.73772177E-02
74	2.98586476E-01	8.64328072E-02
75	2.95306723E-01	8.49431246E-02
76	2.92062675E-01	8.29306571E-02
77	2.88853542E-01	8.04201721E-02
78	2.85679797E-01	7.74393327E-02
79	2.82537777E-01	7.40136281E-02
80	2.79429894E-01	7.01755700E-02
81	2.76354557E-01	6.59549048E-02
82	2.73311130E-01	6.13830944E-02
83	2.70299774E-01	5.64921140E-02
84	2.67319701E-01	5.13142184E-02
85	2.64367759E-01	4.58817256E-02
86	2.61447167E-01	4.02268199E-02
87	2.58556043E-01	3.43813705E-02
88	2.55693957E-01	2.83767692E-02
89	2.52560447E-01	2.22437827E-02
90	2.50053106E-01	1.60124278E-02
91	2.47277519E-01	9.71184595E-03
92	2.44527738E-01	3.37021402E-03
93	2.41804030E-01	-2.95534624E-03
94	2.39107472E-01	-9.32884151E-03
95	2.36436952E-01	-1.56354651E-02
96	2.33792401E-01	-2.19816464E-02
97	2.31173438E-01	-2.80450880E-02
98	2.28579674E-01	-3.41047936E-02
99	2.26010309E-01	-4.00410553E-02
100	2.23466532E-01	-4.59356139E-02

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL AND THE RADIAL WAVE FUNCTION. IONIZATION ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100 BOHR UNITS.

R	PHI(R)	R(R)
101	2.20946541E-01	-5.14713601E-02
102	2.18450543E-01	-5.69326292E-02
103	2.15978254E-01	-6.22050389E-02
104	2.13522395E-01	-6.72755022E-02
105	2.11103697E-01	-7.21322040E-02
106	2.08700898E-01	-7.67645741E-02
107	2.06320743E-01	-8.11632556E-02
108	2.03962983E-01	-8.53200702E-02
109	2.01627376E-01	-8.92279802E-02
110	1.99313687E-01	-9.28810457E-02
111	1.97021684E-01	-9.62743968E-02
112	1.94751146E-01	-9.94041598E-02
113	1.92501853E-01	-1.02267442E-01
114	1.90273590E-01	-1.04862270E-01
115	1.88066153E-01	-1.07187547E-01
116	1.85879336E-01	-1.09243004E-01
117	1.83712943E-01	-1.11029156E-01
118	1.81566779E-01	-1.12547248E-01
119	1.79440657E-01	-1.13799217E-01
120	1.77334390E-01	-1.14797639E-01
121	1.75247799E-01	-1.15515689E-01
122	1.73180707E-01	-1.15987090E-01
123	1.71132941E-01	-1.16206076E-01
124	1.69104334E-01	-1.16177347E-01
125	1.67094718E-01	-1.15906026E-01
126	1.65103933E-01	-1.15397622E-01
127	1.63151920E-01	-1.14657990E-01
128	1.61178224E-01	-1.13697294E-01
129	1.59242993E-01	-1.12509972E-01
130	1.57325977E-01	-1.11114702E-01
131	1.55427073E-01	-1.09514368E-01
132	1.53546013E-01	-1.07716030E-01
133	1.51682780E-01	-1.05726895E-01
134	1.49837126E-01	-1.03554297E-01
135	1.48009124E-01	-1.01205622E-01
136	1.46198433E-01	-9.86883843E-02
137	1.44404991E-01	-9.60100955E-02
138	1.42628670E-01	-9.31783117E-02
139	1.40869345E-01	-9.02005709E-02
140	1.39126893E-01	-8.70844039E-02
141	1.37401190E-01	-8.38373014E-02
142	1.35692118E-01	-8.04667005E-02
143	1.33999559E-01	-7.69799690E-02
144	1.32323328E-01	-7.33843912E-02
145	1.30663520E-01	-6.96871554E-02
146	1.29019813E-01	-6.58953415E-02
147	1.27392167E-01	-6.20159103E-02
148	1.25780473E-01	-5.80556942E-02
149	1.24184625E-01	-5.40213879E-02
150	1.22604515E-01	-4.99195410E-02

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL AND THE RADIAL WAVE FUNCTION. IONIZATION ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100 BOHR UNITS.

R	PHI(R)	R(R)
151	1.21040041E-01	-4.57565509E-02
152	1.19491100E-01	-4.15386570E-02
153	1.17957591E-01	-3.72719253E-02
154	1.16439414E-01	-3.29622941E-02
155	1.14936469E-01	-2.86154701E-02
156	1.13448662E-01	-2.42370258E-02
157	1.11975894E-01	-1.98323465E-02
158	1.10518072E-01	-1.54066392E-02
159	1.09075103E-01	-1.09649309E-02
160	1.07646893E-01	-6.51206799E-03
161	1.06233351E-01	-2.05271628E-03
162	1.04834388E-01	2.40363865E-03
163	1.03449914E-01	6.86769127E-03
164	1.02079841E-01	1.13203146E-02
165	1.00724081E-01	1.57623589E-02
166	9.93825493E-02	2.01906497E-02
167	9.80551593E-02	2.46009364E-02
168	9.67418269E-02	2.89901390E-02
169	9.54424697E-02	3.33548461E-02
170	9.41570017E-02	3.76920120E-02
171	9.28853441E-02	4.19987037E-02
172	9.16274147E-02	4.62721476E-02
173	9.03831332E-02	5.05097262E-02
174	8.91524197E-02	5.47089748E-02
175	8.79351955E-02	5.88675777E-02
176	8.67313892E-02	6.29833644E-02
177	8.55409024E-02	6.70543063E-02
178	8.43636790E-02	7.10785123E-02
179	8.31996358E-02	7.50542252E-02
180	8.20486971E-02	7.89798179E-02
181	8.09107978E-02	8.28537889E-02
182	7.97858335E-02	8.66747590E-02
183	7.86737603E-02	9.04414666E-02
184	7.75744947E-02	9.41527644E-02
185	7.64879639E-02	9.78076149E-02
186	7.54140956E-02	1.01405087E-01
187	7.43528179E-02	1.04944350E-01
188	7.33040595E-02	1.08424675E-01
189	7.22677495E-02	1.11845424E-01
190	7.12439176E-02	1.15206052E-01
191	7.02321936E-02	1.18506093E-01
192	6.92328081E-02	1.21745188E-01
193	6.82455920E-02	1.24923024E-01
194	6.72704766E-02	1.28039386E-01
195	6.63073934E-02	1.31094126E-01
196	6.53562746E-02	1.34087165E-01
197	6.44170526E-02	1.37018491E-01
198	6.34896693E-02	1.39888152E-01
199	6.25740407E-02	1.42696258E-01
200	6.16700973E-02	1.45442973E-01

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL AND THE RADIAL WAVE FUNCTION. IONIZATION ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100 BOHR UNITS.

R	PHI(R)	R(R)
201	6.07777941E-02	1.48128515E-01
202	5.98970551E-02	1.50753154E-01
203	5.90278148E-02	1.53317204E-01
204	5.81700079E-02	1.55821028E-01
205	5.73235696E-02	1.58265026E-01
206	5.64884352E-02	1.60649642E-01
207	5.56645403E-02	1.62975554E-01
208	5.48518209E-02	1.65242675E-01
209	5.40502131E-02	1.67452151E-01
210	5.32596546E-02	1.69604357E-01
211	5.24800785E-02	1.71699395E-01
212	5.17114252E-02	1.73739394E-01
213	5.09536309E-02	1.75723506E-01
214	5.02066328E-02	1.77612903E-01
215	4.94703637E-02	1.79503179E-01
216	4.87447764E-02	1.81350344E-01
217	4.80297939E-02	1.83119824E-01
218	4.73253597E-02	1.84837462E-01
219	4.66314120E-02	1.86504011E-01
220	4.59478897E-02	1.88120235E-01
221	4.52747317E-02	1.89686911E-01
222	4.46117769E-02	1.91204821E-01
223	4.39590649E-02	1.92674757E-01
224	4.33169346E-02	1.94097514E-01
225	4.26845261E-02	1.95473894E-01
226	4.20622791E-02	1.96804701E-01
227	4.14500344E-02	1.98090742E-01
228	4.08477293E-02	1.99332825E-01
229	4.02553071E-02	2.00531759E-01
230	3.96727071E-02	2.01688353E-01
231	3.90999700E-02	2.02803411E-01
232	3.85367366E-02	2.03877739E-01
233	3.79832478E-02	2.04912139E-01
234	3.74393446E-02	2.05907406E-01
235	3.69049682E-02	2.06864334E-01
236	3.63800600E-02	2.07783711E-01
237	3.58645615E-02	2.08666318E-01
238	3.53584141E-02	2.09512931E-01
239	3.48615598E-02	2.10324319E-01
240	3.43739404E-02	2.11101240E-01
241	3.38954978E-02	2.11844450E-01
242	3.34261743E-02	2.12554693E-01
243	3.29659120E-02	2.13232705E-01
244	3.25146532E-02	2.13879213E-01
245	3.20723408E-02	2.14494953E-01
246	3.16389171E-02	2.15080575E-01
247	3.12143248E-02	2.15636034E-01
248	3.07985068E-02	2.16164398E-01
249	3.03914062E-02	2.16663944E-01
250	2.99929659E-02	2.17136137E-01

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL AND THE RADIAL WAVE FUNCTION. IONIZATION ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100 BOHR UNITS.

R	PHI(R)	R(R)
251	2.96031291E-02	2.17531632E-01
252	2.92218392E-02	2.18001072E-01
253	2.88490396E-02	2.18395020E-01
254	2.84846737E-02	2.18764306E-01
255	2.81286851E-02	2.19109329E-01
256	2.77810177E-02	2.19430757E-01
257	2.74416152E-02	2.19729175E-01
258	2.71104216E-02	2.20005158E-01
259	2.67873809E-02	2.20259266E-01
260	2.64724373E-02	2.20492030E-01
261	2.61655747E-02	2.20704043E-01
262	2.58666179E-02	2.20895787E-01
263	2.55756311E-02	2.21067779E-01
264	2.52925139E-02	2.21220528E-01
265	2.50172239E-02	2.21354524E-01
266	2.47496959E-02	2.21470245E-01
267	2.44897767E-02	2.21569157E-01
268	2.42377103E-02	2.21648716E-01
269	2.39931425E-02	2.21712365E-01
270	2.37561136E-02	2.21759534E-01
271	2.35265869E-02	2.21790644E-01
272	2.33044836E-02	2.21806104E-01
273	2.30897632E-02	2.21806309E-01
274	2.28823693E-02	2.21791646E-01
275	2.26822442E-02	2.21762489E-01
276	2.24893360E-02	2.21719202E-01
277	2.23035921E-02	2.21662136E-01
278	2.21249558E-02	2.21591633E-01
279	2.19533739E-02	2.21508024E-01
280	2.17887925E-02	2.21411628E-01
281	2.16311579E-02	2.21302756E-01
282	2.14804134E-02	2.21181706E-01
283	2.13365143E-02	2.21048767E-01
284	2.11993932E-02	2.20904218E-01
285	2.10690145E-02	2.20748328E-01
286	2.09453101E-02	2.20591356E-01
287	2.08282319E-02	2.20403550E-01
288	2.07177244E-02	2.20215151E-01
289	2.06137409E-02	2.20016389E-01
290	2.05162224E-02	2.19807484E-01
291	2.04251191E-02	2.19588649E-01
292	2.03403754E-02	2.19360036E-01
293	2.02619415E-02	2.19121990E-01
294	2.01897641E-02	2.18874545E-01
295	2.01237907E-02	2.18617929E-01
296	2.00639691E-02	2.18352310E-01
297	2.00102470E-02	2.18077848E-01
298	1.99625724E-02	2.17794695E-01
299	1.99208974E-02	2.17502996E-01
300	1.99670061E-02	2.17202886E-01

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL AND THE RADIAL WAVE FUNCTION. IONIZATION ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100 BOHR UNITS.

R	PHI(R)	R(R)
301	1.99341209E-02	2.16894401E-01
302	1.99013438E-02	2.16577666E-01
303	1.98686743E-02	2.16252805E-01
304	1.98361119E-02	2.15919941E-01
305	1.98036561E-02	2.15579198E-01
306	1.97713063E-02	2.15230695E-01
307	1.97390620E-02	2.14874555E-01
308	1.97069227E-02	2.14510896E-01
309	1.96748879E-02	2.14139839E-01
310	1.96429571E-02	2.13761500E-01
311	1.96111297E-02	2.13375996E-01
312	1.95794054E-02	2.12983444E-01
313	1.95477835E-02	2.12583959E-01
314	1.95162636E-02	2.12177656E-01
315	1.94848451E-02	2.11764647E-01
316	1.94535277E-02	2.11345045E-01
317	1.94223108E-02	2.10918961E-01
318	1.93911939E-02	2.10486507E-01
319	1.93601765E-02	2.10047791E-01
320	1.93292582E-02	2.09602923E-01
321	1.92984385E-02	2.09152011E-01
322	1.92677170E-02	2.08695161E-01
323	1.92370931E-02	2.08232479E-01
324	1.92065663E-02	2.07764070E-01
325	1.91761364E-02	2.07290040E-01
326	1.91458027E-02	2.06810490E-01
327	1.91155648E-02	2.06325523E-01
328	1.90854222E-02	2.05835240E-01
329	1.90553746E-02	2.05339743E-01
330	1.90254214E-02	2.04839130E-01
331	1.89955623E-02	2.04333500E-01
332	1.89657967E-02	2.03822951E-01
333	1.89361243E-02	2.03307580E-01
334	1.89065446E-02	2.02787483E-01
335	1.88770571E-02	2.02262754E-01
336	1.88476615E-02	2.01733489E-01
337	1.88183573E-02	2.01199779E-01
338	1.87891441E-02	2.00661717E-01
339	1.87600214E-02	2.00119396E-01
340	1.87309888E-02	1.99572905E-01
341	1.87020460E-02	1.99022333E-01
342	1.86731925E-02	1.98467771E-01
343	1.86444279E-02	1.97909304E-01
344	1.86157518E-02	1.97347022E-01
345	1.85871637E-02	1.96781009E-01
346	1.85586634E-02	1.96211351E-01
347	1.85302502E-02	1.95638132E-01
348	1.85019240E-02	1.95061436E-01
349	1.84736842E-02	1.94481345E-01
350	1.84455305E-02	1.93897941E-01

TABLE V.

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL AND THE RADIAL WAVE FUNCTION. IONIZATION ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100 BOHR UNITS.

R	PHI(R)	R(R)
351	1.84174625E-02	1.93311305E-01
352	1.83894798E-02	1.92721519E-01
353	1.83615819E-02	1.92128657E-01
354	1.83337636E-02	1.91532803E-01
355	1.83060394E-02	1.90934031E-01
356	1.82783940E-02	1.90332420E-01
357	1.82508319E-02	1.89728044E-01
358	1.82233529E-02	1.89120979E-01
359	1.81959563E-02	1.88511299E-01
360	1.81686423E-02	1.87899078E-01
361	1.81414100E-02	1.87284387E-01
362	1.81142572E-02	1.86667299E-01
363	1.80871995E-02	1.86047385E-01
364	1.80602007E-02	1.85426215E-01
365	1.80332922E-02	1.84802359E-01
366	1.80064639E-02	1.84176383E-01
367	1.79797135E-02	1.83548757E-01
368	1.79530459E-02	1.82918348E-01
369	1.79264556E-02	1.82286422E-01
370	1.78999439E-02	1.81652644E-01
371	1.78735105E-02	1.81017079E-01
372	1.78471551E-02	1.80379791E-01
373	1.78208773E-02	1.79740243E-01
374	1.77946768E-02	1.79100398E-01
375	1.77685532E-02	1.78458217E-01
376	1.77425062E-02	1.77814660E-01
377	1.77165354E-02	1.77169689E-01
378	1.76906406E-02	1.76523363E-01
379	1.76648213E-02	1.75875740E-01
380	1.76390773E-02	1.75226879E-01
381	1.76134083E-02	1.74575836E-01
382	1.75878138E-02	1.73925669E-01
383	1.75622936E-02	1.73273433E-01
384	1.75368474E-02	1.72620133E-01
385	1.75114749E-02	1.71965974E-01
386	1.74861755E-02	1.71310859E-01
387	1.74609492E-02	1.70654892E-01
388	1.74357955E-02	1.69998125E-01
389	1.74107143E-02	1.69340610E-01
390	1.73857051E-02	1.68682398E-01
391	1.73607676E-02	1.68023539E-01
392	1.73359016E-02	1.67364082E-01
393	1.73111067E-02	1.66704078E-01
394	1.72863827E-02	1.66043575E-01
395	1.72617291E-02	1.65382619E-01
396	1.72371458E-02	1.64721259E-01
397	1.72126324E-02	1.64059540E-01
398	1.71881886E-02	1.63397510E-01
399	1.71638140E-02	1.62735212E-01
400	1.71395038E-02	1.62072691E-01

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL AND THE RADIAL WAVE FUNCTION. IONIZATION ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100 BOHR UNITS.

R	PHI(R)	R(R)
401	1.71152721E-02	1.61409993E-01
402	1.70911039E-02	1.60747159E-01
403	1.70670049E-02	1.60084233E-01
404	1.70429716E-02	1.59421257E-01
405	1.70190070E-02	1.58758272E-01
406	1.69951097E-02	1.58095320E-01
407	1.69712794E-02	1.57432441E-01
408	1.69475158E-02	1.56769675E-01
409	1.69238187E-02	1.56107060E-01
410	1.69001978E-02	1.55444637E-01
411	1.68766228E-02	1.54782443E-01
412	1.68531233E-02	1.54120514E-01
413	1.68296923E-02	1.53458889E-01
414	1.68063203E-02	1.52797604E-01
415	1.67830162E-02	1.52136695E-01
416	1.67597765E-02	1.51476198E-01
417	1.67366012E-02	1.50816146E-01
418	1.67134899E-02	1.50156575E-01
419	1.66904427E-02	1.49497518E-01
420	1.66674581E-02	1.48839009E-01
421	1.66445372E-02	1.48181080E-01
422	1.66216792E-02	1.47523763E-01
423	1.65988839E-02	1.46867091E-01
424	1.65761511E-02	1.46211094E-01
425	1.65534905E-02	1.45555804E-01
426	1.65308719E-02	1.44901250E-01
427	1.65083247E-02	1.44247462E-01
428	1.64858391E-02	1.43594470E-01
429	1.64634146E-02	1.42942302E-01
430	1.64410511E-02	1.42290987E-01
431	1.64187490E-02	1.41640552E-01
432	1.63965058E-02	1.40991026E-01
433	1.63743236E-02	1.40342434E-01
434	1.63522013E-02	1.39694804E-01
435	1.63301386E-02	1.39048162E-01
436	1.63081355E-02	1.38402532E-01
437	1.62861915E-02	1.37757941E-01
438	1.62643066E-02	1.37114413E-01
439	1.62424807E-02	1.36471972E-01
440	1.62207126E-02	1.35830642E-01
441	1.61990051E-02	1.35190447E-01
442	1.61773517E-02	1.34551409E-01
443	1.61557581E-02	1.33913552E-01
444	1.61342220E-02	1.33276897E-01
445	1.61127433E-02	1.32641466E-01
446	1.60913217E-02	1.32007281E-01
447	1.60699570E-02	1.31374362E-01
448	1.60486499E-02	1.30742731E-01
449	1.60273973E-02	1.30112407E-01
450	1.60062018E-02	1.29483410E-01

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL
AND THE RADIAL WAVE FUNCTION. IONIZATION
ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100
BOHR UNITS.

R	PHI(R)	R(R)
451	1.59850624E-02	1.28855760E-01
452	1.59639787E-02	1.28229475E-01
453	1.59429506E-02	1.27604576E-01
454	1.59219773E-02	1.26981079E-01
455	1.59010601E-02	1.26359002E-01
456	1.58801973E-02	1.25738364E-01
457	1.58593891E-02	1.25119192E-01
458	1.58386354E-02	1.24501472E-01
459	1.58179360E-02	1.23885251E-01
460	1.57972906E-02	1.23270536E-01
461	1.57766990E-02	1.22657341E-01
462	1.57561611E-02	1.22045683E-01
463	1.57356765E-02	1.21435573E-01
464	1.57152451E-02	1.20827038E-01
465	1.56948667E-02	1.20220080E-01
466	1.56745412E-02	1.19614718E-01
467	1.56542681E-02	1.19010965E-01
468	1.56340475E-02	1.18408835E-01
469	1.56138790E-02	1.17808341E-01
470	1.55937625E-02	1.17209496E-01
471	1.55736978E-02	1.16612316E-01
472	1.55536846E-02	1.16016804E-01
473	1.55337228E-02	1.15422982E-01
474	1.55138122E-02	1.14830958E-01
475	1.54939523E-02	1.14240443E-01
476	1.54741436E-02	1.13651749E-01
477	1.54543853E-02	1.13064786E-01
478	1.54346775E-02	1.12479366E-01
479	1.54150198E-02	1.11896098E-01
480	1.53954121E-02	1.11314493E-01
481	1.53758542E-02	1.10734461E-01
482	1.53563460E-02	1.10156310E-01
483	1.53368872E-02	1.09579951E-01
484	1.53174776E-02	1.09005392E-01
485	1.52981172E-02	1.08432643E-01
486	1.52788056E-02	1.07861711E-01
487	1.52595426E-02	1.07292605E-01
488	1.52403281E-02	1.06725333E-01
489	1.52211622E-02	1.06159903E-01
490	1.52020443E-02	1.05596321E-01
491	1.51829743E-02	1.05034596E-01
492	1.51639521E-02	1.04474735E-01
493	1.51449776E-02	1.03916744E-01
494	1.51260504E-02	1.03360630E-01
495	1.51071705E-02	1.02806400E-01
496	1.50883377E-02	1.02254059E-01
497	1.50695519E-02	1.01703613E-01
498	1.50508126E-02	1.01155069E-01
499	1.50321199E-02	1.00608431E-01
500	1.50134736E-02	1.00063705E-01

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GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL AND THE RADIAL WAVE FUNCTION. IONIZATION ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100 BOHR UNITS.

R	PHI(R)	R(R)
501	1.49948735E-02	9.95208963E-02
502	1.49763195E-02	9.89800091E-02
503	1.49578113E-02	9.84410485E-02
504	1.49393488E-02	9.79040188E-02
505	1.49209318E-02	9.73689243E-02
506	1.49025602E-02	9.68357690E-02
507	1.48842337E-02	9.63045569E-02
508	1.48659523E-02	9.57752917E-02
509	1.48477157E-02	9.52479767E-02
510	1.48295238E-02	9.47226153E-02
511	1.48113765E-02	9.41992107E-02
512	1.47932735E-02	9.36777658E-02
513	1.47752147E-02	9.31582833E-02
514	1.47571999E-02	9.26407658E-02
515	1.47392290E-02	9.21252158E-02
516	1.47213018E-02	9.16116355E-02
517	1.47034182E-02	9.11000270E-02
518	1.46855780E-02	9.05903921E-02
519	1.46677810E-02	9.00827327E-02
520	1.46500271E-02	8.95770502E-02
521	1.46323162E-02	8.90733463E-02
522	1.46146480E-02	8.85716220E-02
523	1.45970224E-02	8.80718785E-02
524	1.45794393E-02	8.75741168E-02
525	1.45618984E-02	8.70783378E-02
526	1.45443998E-02	8.65845420E-02
527	1.45269431E-02	8.60927299E-02
528	1.45095283E-02	8.56029021E-02
529	1.44921552E-02	8.51150586E-02
530	1.44748237E-02	8.46291996E-02
531	1.44575336E-02	8.41453250E-02
532	1.44402847E-02	8.36634347E-02
533	1.44230769E-02	8.31835284E-02
534	1.44059101E-02	8.27056055E-02
535	1.43887841E-02	8.22296656E-02
536	1.43716988E-02	8.17557079E-02
537	1.43546540E-02	8.12837316E-02
538	1.43376496E-02	8.08137358E-02
539	1.43206854E-02	8.03457193E-02
540	1.43037614E-02	7.98796811E-02
541	1.42868772E-02	7.94156197E-02
542	1.42700329E-02	7.89535338E-02
543	1.42532283E-02	7.84934218E-02
544	1.42364632E-02	7.80352820E-02
545	1.42197375E-02	7.75791128E-02
546	1.42030510E-02	7.71249122E-02
547	1.41864037E-02	7.66726782E-02
548	1.41697953E-02	7.62224088E-02
549	1.41532258E-02	7.57741018E-02
550	1.41366950E-02	7.53277549E-02

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL AND THE RADIAL WAVE FUNCTION. IONIZATION ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100 BOHR UNITS.

R	PHI(R)	R(R)
551	1.41202028E-02	7.48833657E-02
552	1.41037489E-02	7.44409318E-02
553	1.40873334E-02	7.40004504E-02
554	1.40709561E-02	7.35619190E-02
555	1.40546168E-02	7.31253348E-02
556	1.40383154E-02	7.26906949E-02
557	1.40220518E-02	7.22579963E-02
558	1.40058258E-02	7.18272360E-02
559	1.39896373E-02	7.13984109E-02
560	1.39734862E-02	7.09715177E-02
561	1.39573724E-02	7.05465532E-02
562	1.39412956E-02	7.01235139E-02
563	1.39252559E-02	6.97023964E-02
564	1.39092530E-02	6.92831971E-02
565	1.38932869E-02	6.88659124E-02
566	1.38773574E-02	6.84505386E-02
567	1.38614643E-02	6.80370719E-02
568	1.38456077E-02	6.76255085E-02
569	1.38297872E-02	6.72158443E-02
570	1.38140029E-02	6.68080755E-02
571	1.37982546E-02	6.64021980E-02
572	1.37825421E-02	6.59982075E-02
573	1.37668654E-02	6.55960999E-02
574	1.37512243E-02	6.51958709E-02
575	1.37356187E-02	6.47975162E-02
576	1.37200485E-02	6.44010313E-02
577	1.37045135E-02	6.40064119E-02
578	1.36890137E-02	6.36136532E-02
579	1.36735489E-02	6.32227509E-02
580	1.36581190E-02	6.28337001E-02
581	1.36427239E-02	6.24464963E-02
582	1.36273634E-02	6.20611345E-02
583	1.36120375E-02	6.16776101E-02
584	1.35967461E-02	6.12959181E-02
585	1.35814889E-02	6.09160536E-02
586	1.35662660E-02	6.05380116E-02
587	1.35510771E-02	6.01617871E-02
588	1.35359223E-02	5.97873750E-02
589	1.35208012E-02	5.94147701E-02
590	1.35057140E-02	5.90439672E-02
591	1.34906603E-02	5.86749613E-02
592	1.34756402E-02	5.83077468E-02
593	1.34606535E-02	5.79423186E-02
594	1.34457001E-02	5.75786713E-02
595	1.34307798E-02	5.72167995E-02
596	1.34158927E-02	5.68566976E-02
597	1.34010385E-02	5.64983602E-02
598	1.33862172E-02	5.61417819E-02
599	1.33714286E-02	5.57869569E-02
600	1.33566726E-02	5.54338797E-02

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL AND THE RADIAL WAVE FUNCTION. IONIZATION ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100 BOHR UNITS.

R	PHI(R)	R(R)
601	1.33419492E-02	5.50825447E-02
602	1.33272582E-02	5.47329461E-02
603	1.33125996E-02	5.43850783E-02
604	1.32979731E-02	5.40389355E-02
605	1.32833787E-02	5.36945118E-02
606	1.32688164E-02	5.33518015E-02
607	1.32542859E-02	5.30107987E-02
608	1.32397873E-02	5.26714975E-02
609	1.32253203E-02	5.23338921E-02
610	1.32108849E-02	5.19979764E-02
611	1.31964809E-02	5.16637444E-02
612	1.31821084E-02	5.13311903E-02
613	1.31677671E-02	5.10003079E-02
614	1.31534570E-02	5.06710912E-02
615	1.31391780E-02	5.03435340E-02
616	1.31249299E-02	5.00176304E-02
617	1.31107127E-02	4.96933741E-02
618	1.30965262E-02	4.93707590E-02
619	1.30823705E-02	4.90497789E-02
620	1.30682453E-02	4.87304276E-02
621	1.30541506E-02	4.84126989E-02
622	1.30400862E-02	4.80965866E-02
623	1.30260521E-02	4.77820843E-02
624	1.30120482E-02	4.74691857E-02
625	1.29980744E-02	4.71578847E-02
626	1.29841305E-02	4.68481748E-02
627	1.29702165E-02	4.65400497E-02
628	1.29563324E-02	4.62335030E-02
629	1.29424779E-02	4.59285284E-02
630	1.29286530E-02	4.56251195E-02
631	1.29148576E-02	4.53232699E-02
632	1.29010916E-02	4.50229731E-02
633	1.28873550E-02	4.47242228E-02
634	1.28736475E-02	4.44270124E-02
635	1.28599692E-02	4.41313355E-02
636	1.28463199E-02	4.38371857E-02
637	1.28326996E-02	4.35445564E-02
638	1.28191081E-02	4.32534411E-02
639	1.28055454E-02	4.29638334E-02
640	1.27920114E-02	4.26757267E-02
641	1.27785059E-02	4.23891144E-02
642	1.27650289E-02	4.21039902E-02
643	1.27515803E-02	4.18203473E-02
644	1.27381600E-02	4.15381793E-02
645	1.27247680E-02	4.12574796E-02
646	1.27114040E-02	4.09782417E-02
647	1.26980682E-02	4.07004588E-02
648	1.26847602E-02	4.04241245E-02
649	1.26714801E-02	4.01492322E-02
650	1.26582278E-02	3.98757753E-02

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL AND THE RADIAL WAVE FUNCTION. IONIZATION ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100 BOHR UNITS.

R	PHI(R)	R(R)
651	1.26582278E-02	3.96037471E-02
652	1.26582278E-02	3.93331399E-02
653	1.26582278E-02	3.90639457E-02
654	1.26582278E-02	3.87961567E-02
655	1.26582278E-02	3.85297651E-02
656	1.26582278E-02	3.82647632E-02
657	1.26582278E-02	3.80011430E-02
658	1.26582278E-02	3.77388969E-02
659	1.26582278E-02	3.74780172E-02
660	1.26582278E-02	3.72184960E-02
661	1.26582278E-02	3.69603258E-02
662	1.26582278E-02	3.67034988E-02
663	1.26582278E-02	3.64480074E-02
664	1.26582278E-02	3.61938440E-02
665	1.26582278E-02	3.59410008E-02
666	1.26582278E-02	3.56894705E-02
667	1.26582278E-02	3.54392453E-02
668	1.26582278E-02	3.51903176E-02
669	1.26582278E-02	3.49426801E-02
670	1.26582278E-02	3.46963251E-02
671	1.26582278E-02	3.44512452E-02
672	1.26582278E-02	3.42074329E-02
673	1.26582278E-02	3.39648807E-02
674	1.26582278E-02	3.37235812E-02
675	1.26582278E-02	3.34835271E-02
676	1.26582278E-02	3.32447108E-02
677	1.26582278E-02	3.30071250E-02
678	1.26582278E-02	3.27707624E-02
679	1.26582278E-02	3.25356157E-02
680	1.26582278E-02	3.23016774E-02
681	1.26582278E-02	3.20689405E-02
682	1.26582278E-02	3.18373975E-02
683	1.26582278E-02	3.16070412E-02
684	1.26582278E-02	3.13778644E-02
685	1.26582278E-02	3.11498599E-02
686	1.26582278E-02	3.09230205E-02
687	1.26582278E-02	3.06973390E-02
688	1.26582278E-02	3.04728083E-02
689	1.26582278E-02	3.02494213E-02
690	1.26582278E-02	3.00271708E-02
691	1.26582278E-02	2.98060497E-02
692	1.26582278E-02	2.95860511E-02
693	1.26582278E-02	2.93671678E-02
694	1.26582278E-02	2.91493928E-02
695	1.26582278E-02	2.89327191E-02
696	1.26582278E-02	2.87171397E-02
697	1.26582278E-02	2.85026477E-02
698	1.26582278E-02	2.82892361E-02
699	1.26582278E-02	2.80768980E-02
700	1.26582278E-02	2.78656264E-02

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL AND THE RADIAL WAVE FUNCTION. IONIZATION ENERGY=.666 RYDBERGS. R IS IN JNITS OF 1/100 BOHR UNITS.

R	PHI(R)	R(R)
701	1.26582278E-02	2.76554146E-02
702	1.26582278E-02	2.74462555E-02
703	1.26582278E-02	2.72381425E-02
704	1.26582278E-02	2.70310686E-02
705	1.26582278E-02	2.68250270E-02
706	1.26582278E-02	2.66200110E-02
707	1.26582278E-02	2.64160138E-02
708	1.26582278E-02	2.62130286E-02
709	1.26582278E-02	2.60110487E-02
710	1.26582278E-02	2.58100675E-02
711	1.26582278E-02	2.56100781E-02
712	1.26582278E-02	2.54110739E-02
713	1.26582278E-02	2.52130484E-02
714	1.26582278E-02	2.50159948E-02
715	1.26582278E-02	2.48199065E-02
716	1.26582278E-02	2.46247770E-02
717	1.26582278E-02	2.44305996E-02
718	1.26582278E-02	2.42373679E-02
719	1.26582278E-02	2.40450752E-02
720	1.26582278E-02	2.38537151E-02
721	1.26582278E-02	2.36632810E-02
722	1.26582278E-02	2.34737665E-02
723	1.26582278E-02	2.32851651E-02
724	1.26582278E-02	2.30974704E-02
725	1.26582278E-02	2.29106759E-02
726	1.26582278E-02	2.27247753E-02
727	1.26582278E-02	2.25397621E-02
728	1.26582278E-02	2.23556300E-02
729	1.26582278E-02	2.21723726E-02
730	1.26582278E-02	2.19899835E-02
731	1.26582278E-02	2.18084566E-02
732	1.26582278E-02	2.16277854E-02
733	1.26582278E-02	2.14479637E-02
734	1.26582278E-02	2.12689852E-02
735	1.26582278E-02	2.10908437E-02
736	1.26582278E-02	2.09135330E-02
737	1.26582278E-02	2.07370468E-02
738	1.26582278E-02	2.05613789E-02
739	1.26582278E-02	2.03865232E-02
740	1.26582278E-02	2.02124735E-02
741	1.26582278E-02	2.00392237E-02
742	1.26582278E-02	1.98667676E-02
743	1.26582278E-02	1.96950992E-02
744	1.26582278E-02	1.95242123E-02
745	1.26582278E-02	1.93541009E-02
746	1.26582278E-02	1.91847589E-02
747	1.26582278E-02	1.90161802E-02
748	1.26582278E-02	1.88483589E-02
749	1.26582278E-02	1.86812889E-02
750	1.26582278E-02	1.85149643E-02

TABLE V

GOLD

PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL AND THE RADIAL WAVE FUNCTION. IONIZATION ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100 BOHR UNITS.

R	PHI(R)	R(R)
751	1.26582278E-02	1.83493791E-02
752	1.26582278E-02	1.81845272E-02
753	1.26582278E-02	1.80204028E-02
754	1.26582278E-02	1.78569999E-02
755	1.26582278E-02	1.76943127E-02
756	1.26582278E-02	1.75323351E-02
757	1.26582278E-02	1.73710614E-02
758	1.26582278E-02	1.72104857E-02
759	1.26582278E-02	1.70506021E-02
760	1.26582278E-02	1.68914047E-02
761	1.26582278E-02	1.67328878E-02
762	1.26582278E-02	1.65750456E-02
763	1.26582278E-02	1.64178722E-02
764	1.26582278E-02	1.62613619E-02
765	1.26582278E-02	1.61055089E-02
766	1.26582278E-02	1.59503075E-02
767	1.26582278E-02	1.57957519E-02
768	1.26582278E-02	1.56418365E-02
769	1.26582278E-02	1.54885554E-02
770	1.26582278E-02	1.53359031E-02
771	1.26582278E-02	1.51838738E-02
772	1.26582278E-02	1.50324618E-02
773	1.26582278E-02	1.48816616E-02
774	1.26582278E-02	1.47314675E-02
775	1.26582278E-02	1.45818738E-02
776	1.26582278E-02	1.44328750E-02
777	1.26582278E-02	1.42844654E-02
778	1.26582278E-02	1.41366395E-02
779	1.26582278E-02	1.39893916E-02
780	1.26582278E-02	1.38427163E-02
781	1.26582278E-02	1.36966080E-02
782	1.26582278E-02	1.35510611E-02
783	1.26582278E-02	1.34060702E-02
784	1.26582278E-02	1.32616297E-02
785	1.26582278E-02	1.31177341E-02
786	1.26582278E-02	1.29743779E-02
787	1.26582278E-02	1.28315557E-02
788	1.26582278E-02	1.26892619E-02
789	1.26582278E-02	1.25474912E-02
790	1.26582278E-02	1.24062382E-02
791	1.26582278E-02	1.22654973E-02
792	1.26582278E-02	1.21252631E-02
793	1.26582278E-02	1.19855303E-02
794	1.26582278E-02	1.18462934E-02
795	1.26582278E-02	1.17075472E-02
796	1.26582278E-02	1.15692861E-02
797	1.26582278E-02	1.14315048E-02
798	1.26582278E-02	1.12941980E-02
799	1.26582278E-02	1.11573604E-02
800	1.26582278E-02	1.10209865E-02

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                          TABLE V

                           GOLD

        PHI(R) CONTRIBUTIONS TO THE EFFECTIVE POTENTIAL
         AND THE RADIAL WAVE FUNCTION. IONIZATION
         ENERGY=.666 RYDBERGS. R IS IN UNITS OF 1/100
         BOHR UNITS.

       R                  PHI(R)                       R(R)

      801            1.26582278E-02               1.08850711E-02
      802            1.26582278E-02               1.07496089E-02
      803            1.26582278E-02               1.06145945E-02
      804            1.26582278E-02               1.04800227E-02
      805            1.26582278E-02               1.03458882E-02
      806            1.26582278E-02               1.02121856E-02
      807            1.26582278E-02               1.00789098E-02
      808            1.26582278E-02               9.94605545E-03
      809            1.26582278E-02               9.81361731E-03
      810            1.26582278E-02               9.68159016E-03
      811            1.26582278E-02               9.54996874E-03
      812            1.26582278E-02               9.41874784E-03
      813            1.26582278E-02               9.28792224E-03
      814            1.26582278E-02               9.15748674E-03
      815            1.26582278E-02               9.02743612E-03
      816            1.26582278E-02               8.89776519E-03
      817            1.26582278E-02               8.76846878E-03
      818            1.26582278E-02               8.63954169E-03
      819            1.26582278E-02               8.51097876E-03
      820            1.26582278E-02               8.38277483E-03
      821            1.26582278E-02               8.25492473E-03
      822            1.26582278E-02               8.12742331E-03
      823            1.26582278E-02               8.00026543E-03
      824            1.26582278E-02               7.87344596E-03
      825            1.26582278E-02               7.74695975E-03
      826            1.26582278E-02               7.62080168E-03
      827            1.26582278E-02               7.49496664E-03
      828            1.26582278E-02               7.36944950E-03
      829            1.26582278E-02               7.24424517E-03
      830            1.26582278E-02               7.11934853E-03
TIME,   1 MINUTES AND    4 SECONDS
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TABLE VI

GOLD

VALUES FOR PSI(R) AND PSI(R) PSI(R)*. R IN UNITS OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666 RYDBERGS.

R	PSI(R)	PSI(R)PSI(R)*
1	7.63658744E-01	5.83174678E-01
2	1.40284349E+00	5.83174678E-01
3	9.90852310E-01	5.83174678E-01
4	4.66533645E-01	5.83174678E-01
5	3.59848971E-02	5.83174678E-01
6	-2.58283165E-01	5.83174678E-01
7	-4.25144424E-01	5.83174678E-01
8	-4.89413706E-01	5.83174678E-01
9	-4.78556795E-01	5.83174678E-01
10	-4.17480428E-01	5.83174678E-01
11	-3.26822316E-01	5.83174678E-01
12	-2.22654629E-01	5.83174678E-01
13	-1.16857130E-01	5.83174678E-01
14	-1.77268191E-02	5.83174678E-01
15	6.93608359E-02	5.83174678E-01
16	1.41327510E-01	5.83174678E-01
17	1.96841754E-01	5.83174678E-01
18	2.35854019E-01	5.83174678E-01
19	2.59216815E-01	5.83174678E-01
20	2.68378276E-01	5.83174678E-01
21	2.65146243E-01	5.83174678E-01
22	2.51505563E-01	5.83174678E-01
23	2.29483073E-01	5.83174678E-01
24	2.01050120E-01	5.83174678E-01
25	1.68055230E-01	5.83174678E-01
26	1.32180479E-01	5.83174678E-01
27	9.49161975E-02	5.83174678E-01
28	5.75495744E-02	5.83174678E-01
29	2.11635936E-02	5.83174678E-01
30	-1.33566016E-02	5.83174678E-01
31	-4.53121926E-02	5.83174678E-01
32	-7.41758143E-02	5.83174678E-01
33	-9.95747180E-02	5.83174678E-01
34	-1.21273023E-01	5.83174678E-01
35	-1.39153846E-01	5.83174678E-01
36	-1.53201830E-01	5.83174678E-01
37	-1.63486841E-01	5.83174678E-01
38	-1.70148009E-01	5.83174678E-01
39	-1.73380029E-01	5.83174678E-01
40	-1.73420430E-01	5.83174678E-01
41	-1.70537799E-01	5.83174678E-01
42	-1.65021995E-01	5.83174678E-01
43	-1.57175632E-01	5.83174678E-01
44	-1.47306497E-01	5.83174678E-01
45	-1.35721350E-01	5.83174678E-01
46	-1.22720798E-01	5.83174678E-01
47	-1.08595022E-01	5.83174678E-01
48	-9.36205320E-02	5.83174678E-01
49	-7.80575737E-02	5.83174678E-01
50	-6.21482701E-02	5.83174678E-01

TABLE VI

GOLD

VALUES FOR PSI(R) AND PSI(R) PSI(R)*. R IN UNITS OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666 RYDBERGS.

R	PSI(R)	PSI(R)PSI(R)*
51	-4.61153389E-02	5.83174678E-01
52	-3.01613211E-02	5.83174678E-01
53	-1.44682421E-02	5.83174678E-01
54	8.02364129E-04	5.83174678E-01
55	1.55091306E-02	5.83174678E-01
56	2.95302871E-02	5.83174678E-01
57	4.27628951E-02	5.83174678E-01
58	5.51219316E-02	5.83174678E-01
59	6.65392594E-02	5.83174678E-01
60	7.69625176E-02	5.83174678E-01
61	8.63539606E-02	5.83174678E-01
62	9.46892699E-02	5.83174678E-01
63	1.01956359E-01	5.83174678E-01
64	1.08154199E-01	5.83174678E-01
65	1.13291607E-01	5.83174678E-01
66	1.17386[illegible]E-01	5.83174678E-01
67	1.204633[illegible]E-01	5.83174678E-01
68	1.225548[illegible]7[illegible]-01	5.83174678E-01
69	1.23698435E-01	5.83174678E-01
70	1.23936440E-01	5.83174678E-01
71	1.23315165E-01	5.83174678E-01
72	1.218849[illegible]E-01	5.83174678E-01
73	1.19694819E-01	5.83174678E-01
74	1.16801091E-01	5.83174678E-01
75	1.13257499E-01	5.83174678E-01
76	1.09119226E-01	5.83174678E-01
77	1.0444173[illegible]E-01	5.83174678E-01
78	9.92799778E-02	5.83174678E-01
79	9.36881369E-02	5.83174678E-01
80	8.77194625E-02	5.83174678E-01
81	8.14258084E-02	5.83174678E-01
82	7.43574322E-02	5.83174678E-01
83	6.80627880E-02	5.83174678E-01
84	6.10883552E-02	5.83174678E-01
85	5.39785008E-02	5.83174678E-01
86	4.67753720E-02	5.83174678E-01
87	3.95188166E-02	5.83174678E-01
88	3.22467286E-02	5.83174678E-01
89	2.49930154E-02	5.83174678E-01
90	1.77915864E-02	5.83174678E-01
91	1.06723582E-02	5.83174678E-01
92	3.66327633E-03	5.83174678E-01
93	-3.21004972E-03	5.83174678E-01
94	-9.92429948E-03	5.83174678E-01
95	-1.64583843E-02	5.83174678E-01
96	-2.27933916E-02	5.83174678E-01
97	-2.89124619E-02	5.83174678E-01
98	-3.48008098E-02	5.83174678E-01
99	-4.04455407E-02	5.83174678E-01
100	-4.58356139E-02	5.83174678E-01

TABLE VI

GOLD

VALUES FOR PSI(R) AND PSI(R) PSI(R)*. R IN UNITS OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666 RYDBERGS.

R	PSI(R)	PSI(R)PSI(R)*
101	-5.09617427E-02	5.83174678E-01
102	-5.58163031E-02	5.83174678E-01
103	-6.03932417E-02	5.83174678E-01
104	-6.46879829E-02	5.83174678E-01
105	-6.86973372E-02	5.83174678E-01
106	-7.24194096E-02	5.83174678E-01
107	-7.58535029E-02	5.83174678E-01
108	-7.90000650E-02	5.83174678E-01
109	-8.18605323E-02	5.83174678E-01
110	-8.44373170E-02	5.83174678E-01
111	-8.67336908E-02	5.83174678E-01
112	-8.87537141E-02	5.83174678E-01
113	-9.05021609E-02	5.83174678E-01
114	-9.19844473E-02	5.83174678E-01
115	-9.32065626E-02	5.83174678E-01
116	-9.41750038E-02	5.83174678E-01
117	-9.48967141E-02	5.83174678E-01
118	-9.53790236E-02	5.83174678E-01
119	-9.56295959E-02	5.83174678E-01
120	-9.56563661E-02	5.83174678E-01
121	-9.54675113E-02	5.83174678E-01
122	-9.50713852E-02	5.83174678E-01
123	-9.44764949E-02	5.83174678E-01
124	-9.36914091E-02	5.83174678E-01
125	-9.27248209E-02	5.83174678E-01
126	-9.15854143E-02	5.83174678E-01
127	-9.02818817E-02	5.83174678E-01
128	-8.88228857E-02	5.83174678E-01
129	-8.72170324E-02	5.83174678E-01
130	-8.54728474E-02	5.83174678E-01
131	-8.35987539E-02	5.83174678E-01
132	-8.16030528E-02	5.83174678E-01
133	-7.94939057E-02	5.83174678E-01
134	-7.72793184E-02	5.83174678E-01
135	-7.49671276E-02	5.83174678E-01
136	-7.25649885E-02	5.83174678E-01
137	-7.00803639E-02	5.83174678E-01
138	-6.75205158E-02	5.83174678E-01
139	-6.48924971E-02	5.83174678E-01
140	-6.22031456E-02	5.83174678E-01
141	-5.94590790E-02	5.83174678E-01
142	-5.66666905E-02	5.83174678E-01
143	-5.38321461E-02	5.83174678E-01
144	-5.09613328E-02	5.83174678E-01
145	-4.80601073E-02	5.83174678E-01
146	-4.51337955E-02	5.83174678E-01
147	-4.21876941E-02	5.83174678E-01
148	-3.92268204E-02	5.83174678E-01
149	-3.62559651E-02	5.83174678E-01
150	-3.32796940E-02	5.83174678E-01

TABLE VI

GOLD

VALUES FOR PSI(R) AND PSI(R) PSI(R)*. R IN UNITS OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666 RYDBERGS.

R	PSI(R)	PSI(R)PSI(R)*
151	-3.03023516E-02	5.83174678E-01
152	-2.73280638E-02	5.83174678E-01
153	-2.43607420E-02	5.83174678E-01
154	-2.14040871E-02	5.83174678E-01
155	-1.84615936E-02	5.83174678E-01
156	-1.55365550E-02	5.83174678E-01
157	-1.26320678E-02	5.83174678E-01
158	-9.75103744E-03	5.83174678E-01
159	-6.89618288E-03	5.83174678E-01
160	-4.07004243E-03	5.83174678E-01
161	-1.27497905E-03	5.83174678E-01
162	1.48681398E-03	5.83174678E-01
163	4.21370753E-03	5.83174678E-01
164	6.90263084E-03	5.83174678E-01
165	9.55306596E-03	5.83174678E-01
166	1.21639420E-02	5.83174678E-01
167	1.47311296E-02	5.83174678E-01
168	1.72560351E-02	5.83174678E-01
169	1.97365953E-02	5.83174678E-01
170	2.21717718E-02	5.83174678E-01
171	2.45606454E-02	5.83174678E-01
172	2.69024114E-02	5.83174678E-01
173	2.91963735E-02	5.83174678E-01
174	3.14419395E-02	5.83174678E-01
175	3.36386158E-02	5.83174678E-01
176	3.57860025E-02	5.83174678E-01
177	3.78837889E-02	5.83174678E-01
178	3.99317485E-02	5.83174678E-01
179	4.19297348E-02	5.83174678E-01
180	4.38776756E-02	5.83174678E-01
181	4.57755740E-02	5.83174678E-01
182	4.76234939E-02	5.83174678E-01
183	4.94215664E-02	5.83174678E-01
184	5.11699806E-02	5.83174678E-01
185	5.28689810E-02	5.83174678E-01
186	5.45198638E-02	5.83174678E-01
187	5.61199735E-02	5.83174678E-01
188	5.76726996E-02	5.83174678E-01
189	5.91774732E-02	5.83174678E-01
190	6.06347641E-02	5.83174678E-01
191	6.20450776E-02	5.83174678E-01
192	6.34089519E-02	5.83174678E-01
193	6.47269553E-02	5.83174678E-01
194	6.59996834E-02	5.83174678E-01
195	6.72277569E-02	5.83174678E-01
196	6.84118190E-02	5.83174678E-01
197	6.95525535E-02	5.83174678E-01
198	7.06505819E-02	5.83174678E-01
199	7.17066622E-02	5.83174678E-01
200	7.27214863E-02	5.83174678E-01

TABLE VI

GOLD

VALUES FOR PSI(R) AND PSI(R) PSI(R)*. R IN UNITS OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666 RYDBERGS.

R	PSI(R)	PSI(R)PSI(R)*
201	7.36957737E-02	5.83174678E-01
202	7.46302741E-02	5.83174678E-01
203	7.55257165E-02	5.83174678E-01
204	7.63828568E-02	5.83174678E-01
205	7.72024519E-02	5.83174678E-01
206	7.79852632E-02	5.83174678E-01
207	7.87320551E-02	5.83174678E-01
208	7.94433939E-02	5.83174678E-01
209	8.01206465E-02	5.83174678E-01
210	8.07639795E-02	5.83174678E-01
211	8.13743579E-02	5.83174678E-01
212	8.19525444E-02	5.83174678E-01
213	8.24992925E-02	5.83174678E-01
214	8.30153752E-02	5.83174678E-01
215	8.35015250E-02	5.83174678E-01
216	8.39584924E-02	5.83174678E-01
217	8.43870158E-02	5.83174678E-01
218	8.47878266E-02	5.83174678E-01
219	8.51616487E-02	5.83174678E-01
220	8.55091978E-02	5.83174678E-01
221	8.58311814E-02	5.83174678E-01
222	8.61282979E-02	5.83174678E-01
223	8.64012369E-02	5.83174678E-01
224	8.66506759E-02	5.83174678E-01
225	8.68772861E-02	5.83174678E-01
226	8.70817260E-02	5.83174678E-01
227	8.72646439E-02	5.83174678E-01
228	8.74266777E-02	5.83174678E-01
229	8.75684539E-02	5.83174678E-01
230	8.76905881E-02	5.83174678E-01
231	8.77936845E-02	5.83174678E-01
232	8.78783360E-02	5.83174678E-01
233	8.79451239E-02	5.83174678E-01
234	8.79946180E-02	5.83174678E-01
235	8.80273763E-02	5.83174678E-01
236	8.80439454E-02	5.83174678E-01
237	8.80448601E-02	5.83174678E-01
238	8.80306434E-02	5.83174678E-01
239	8.80018067E-02	5.83174678E-01
240	8.79588501E-02	5.83174678E-01
241	8.79022615E-02	5.83174678E-01
242	8.78325179E-02	5.83174678E-01
243	8.77500845E-02	5.83174678E-01
244	8.76554151E-02	5.83174678E-01
245	8.75489524E-02	5.83174678E-01
246	8.74311279E-02	5.83174678E-01
247	8.73023618E-02	5.83174678E-01
248	8.71630637E-02	5.83174678E-01
249	8.70136320E-02	5.83174678E-01
250	8.68544547E-02	5.83174678E-01

TABLE VI

GOLD

VALUES FOR PSI(R) AND PSI(R) PSI(R)*. R IN UNITS OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666 RYDBERGS.

R	PSI(R)	PSI(R)PSI(R)*
251	8.66859090E-02	5.83174678E-01
252	8.65083619E-02	5.83174678E-01
253	8.63221699E-02	5.83174678E-01
254	8.61276795E-02	5.83174678E-01
255	8.59252271E-02	5.83174678E-01
256	8.57151395E-02	5.83174678E-01
257	8.54977336E-02	5.83174678E-01
258	8.52733169E-02	5.83174678E-01
259	8.50421876E-02	5.83174678E-01
260	8.48046346E-02	5.83174678E-01
261	8.45609380E-02	5.83174678E-01
262	8.43113689E-02	5.83174678E-01
263	8.40561399E-02	5.83174678E-01
264	8.37956546E-02	5.83174678E-01
265	8.35300090E-02	5.83174678E-01
266	8.32594904E-02	5.83174678E-01
267	8.29843285E-02	5.83174678E-01
268	8.27047448E-02	5.83174678E-01
269	8.24209534E-02	5.83174678E-01
270	8.21331608E-02	5.83174678E-01
271	8.18415662E-02	5.83174678E-01
272	8.15463617E-02	5.83174678E-01
273	8.12477323E-02	5.83174678E-01
274	8.09458563E-02	5.83174678E-01
275	8.06409052E-02	5.83174678E-01
276	8.03330441E-02	5.83174678E-01
277	8.00224816E-02	5.83174678E-01
278	7.97092204E-02	5.83174678E-01
279	7.93935568E-02	5.83174678E-01
280	7.90755815E-02	5.83174678E-01
281	7.87554291E-02	5.83174678E-01
282	7.84332290E-02	5.83174678E-01
283	7.81091050E-02	5.83174678E-01
284	7.77831735E-02	5.83174678E-01
285	7.74555538E-02	5.83174678E-01
286	7.71263482E-02	5.83174678E-01
287	7.67956622E-02	5.83174678E-01
288	7.64635943E-02	5.83174678E-01
289	7.61302384E-02	5.83174678E-01
290	7.57956942E-02	5.83174678E-01
291	7.54600169E-02	5.83174678E-01
292	7.51233173E-02	5.83174678E-01
293	7.47856691E-02	5.83174678E-01
294	7.44471243E-02	5.83174678E-01
295	7.41077727E-02	5.83174678E-01
296	7.37676724E-02	5.83174678E-01
297	7.34268849E-02	5.83174678E-01
298	7.30854633E-02	5.83174678E-01
299	7.27434769E-02	5.83174678E-01
300	7.24009621E-02	5.83174678E-01

TABLE VI

GOLD

VALUES FOR PSI(R) AND PSI(R) PSI(R)*. R IN UNITS OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666 RYDBERGS.

R	PSI(R)	PSI(R)PSI(R)*
301	7.20579406E-02	5.83174678E-01
302	7.17144589E-02	5.83174678E-01
303	7.13705627E-02	5.83174678E-01
304	7.10262965E-02	5.83174678E-01
305	7.06817041E-02	5.83174678E-01
306	7.03368285E-02	5.83174678E-01
307	6.99917117E-02	5.83174678E-01
308	6.96463950E-02	5.83174678E-01
309	6.93009187E-02	5.83174678E-01
310	6.89553224E-02	5.83174678E-01
311	6.86096450E-02	5.83174678E-01
312	6.82639244E-02	5.83174678E-01
313	6.79181979E-02	5.83174678E-01
314	6.75725018E-02	5.83174678E-01
315	6.72268770E-02	5.83174678E-01
316	6.68813432E-02	5.83174678E-01
317	6.65359499E-02	5.83174678E-01
318	6.61907254E-02	5.83174678E-01
319	6.58457026E-02	5.83174678E-01
320	6.55009136E-02	5.83174678E-01
321	6.51563897E-02	5.83174678E-01
322	6.48121617E-02	5.83174678E-01
323	6.44682597E-02	5.83174678E-01
324	6.41247131E-02	5.83174678E-01
325	6.37815506E-02	5.83174678E-01
326	6.34389005E-02	5.83174678E-01
327	6.30964901E-02	5.83174678E-01
328	6.27546464E-02	5.83174678E-01
329	6.24132956E-02	5.83174678E-01
330	6.20724636E-02	5.83174678E-01
331	6.17321752E-02	5.83174678E-01
332	6.13924552E-02	5.83174678E-01
333	6.10533274E-02	5.83174678E-01
334	6.07148153E-02	5.83174678E-01
335	6.03769416E-02	5.83174678E-01
336	6.00397287E-02	5.83174678E-01
337	5.97031985E-02	5.83174678E-01
338	5.93673720E-02	5.83174678E-01
339	5.90322702E-02	5.83174678E-01
340	5.86979131E-02	5.83174678E-01
341	5.83643206E-02	5.83174678E-01
342	5.80315119E-02	5.83174678E-01
343	5.76995056E-02	5.83174678E-01
344	5.73683203E-02	5.83174678E-01
345	5.70379736E-02	5.83174678E-01
346	5.67084828E-02	5.83174678E-01
347	5.63798651E-02	5.83174678E-01
348	5.60521367E-02	5.83174678E-01
349	5.57253137E-02	5.83174678E-01
350	5.53994117E-02	5.83174678E-01

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GOLD

VALUES FOR PSI(R) AND PSI(R) PSI(R)*. R IN UNITS OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666 RYDBERGS.

R	PSI(R)	PSI(R)PSI(R)*
351	5.50744460E-02	5.83174678E-01
352	5.47504312E-02	5.83174678E-01
353	5.44273817E-02	5.83174678E-01
354	5.41053115E-02	5.83174678E-01
355	5.37842342E-02	5.83174678E-01
356	5.34641629E-02	5.83174678E-01
357	5.31451104E-02	5.83174678E-01
358	5.28270892E-02	5.83174678E-01
359	5.25101112E-02	5.83174678E-01
360	5.21941883E-02	5.83174678E-01
361	5.18793316E-02	5.83174678E-01
362	5.15655523E-02	5.83174678E-01
363	5.12528610E-02	5.83174678E-01
364	5.09412679E-02	5.83174678E-01
365	5.06307830E-02	5.83174678E-01
366	5.03214161E-02	5.83174678E-01
367	5.00131763E-02	5.83174678E-01
368	4.97060729E-02	5.83174678E-01
369	4.94001144E-02	5.83174678E-01
370	4.90953092E-02	5.83174678E-01
371	4.87916656E-02	5.83174678E-01
372	4.84891912E-02	5.83174678E-01
373	4.81878937E-02	5.83174678E-01
374	4.78877802E-02	5.83174678E-01
375	4.75888577E-02	5.83174678E-01
376	4.72911531E-02	5.83174678E-01
377	4.69946126E-02	5.83174678E-01
378	4.66993024E-02	5.83174678E-01
379	4.64052035E-02	5.83174678E-01
380	4.61123365E-02	5.83174678E-01
381	4.58206919E-02	5.83174678E-01
382	4.55302798E-02	5.83174678E-01
383	4.52411051E-02	5.83174678E-01
384	4.49531726E-02	5.83174678E-01
385	4.46664956E-02	5.83174678E-01
386	4.43810515E-02	5.83174678E-01
387	4.40968714E-02	5.83174678E-01
388	4.38139498E-02	5.83174678E-01
389	4.35322905E-02	5.83174678E-01
390	4.32519968E-02	5.83174678E-01
391	4.29727720E-02	5.83174678E-01
392	4.26949190E-02	5.83174678E-01
393	4.24183405E-02	5.83174678E-01
394	4.21430392E-02	5.83174678E-01
395	4.18690175E-02	5.83174678E-01
396	4.15962775E-02	5.83174678E-01
397	4.13248212E-02	5.83174678E-01
398	4.10546506E-02	5.83174678E-01
399	4.07857674E-02	5.83174678E-01
400	4.05181729E-02	5.83174678E-01

TABLE VI

GOLD

VALUES FOR PSI(R) AND PSI(R) PSI(R)*. R IN UNITS OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666 RYDBERGS.

R	PSI(R)	PSI(R)PSI(R)*
401	4.02518685E-02	5.83174678E-01
402	3.99868555E-02	5.83174678E-01
403	3.97231347E-02	5.83174678E-01
404	3.94607071E-02	5.83174678E-01
405	3.91995734E-02	5.83174678E-01
406	3.89397340E-02	5.83174678E-01
407	3.86811894E-02	5.83174678E-01
408	3.84239398E-02	5.83174678E-01
409	3.81679854E-02	5.83174678E-01
410	3.79133260E-02	5.83174678E-01
411	3.76599616E-02	5.83174678E-01
412	3.74078917E-02	5.83174678E-01
413	3.71571160E-02	5.83174678E-01
414	3.69076339E-02	5.83174678E-01
415	3.66594447E-02	5.83174678E-01
416	3.64125476E-02	5.83174678E-01
417	3.61669416E-02	5.83174678E-01
418	3.59226[illegible]E-02	5.83174678E-01
419	3.56795987E-02	5.83174678E-01
420	3.54378593E-02	5.83174678E-01
421	3.51974062E-02	5.83174678E-01
422	3.49582378E-02	5.83174678E-01
423	3.47203525E-02	5.83174678E-01
424	3.44837486E-02	5.83174678E-01
425	3.42484244E-02	5.83174678E-01
426	3.40143778E-02	5.83174678E-01
427	3.37816070E-02	5.83174678E-01
428	3.35501027E-02	5.83174678E-01
429	3.33198839E-02	5.83174678E-01
430	3.30909272E-02	5.83174678E-01
431	3.28632372E-02	5.83174678E-01
432	3.26368115E-02	5.83174678E-01
433	3.24116477E-02	5.83174678E-01
434	3.21877429E-02	5.83174678E-01
435	3.19650947E-02	5.83174678E-01
436	3.17437001E-02	5.83174678E-01
437	3.15235563E-02	5.83174678E-01
438	3.13046605E-02	5.83174678E-01
439	3.10870095E-02	5.83174678E-01
440	3.08706005E-02	5.83174678E-01
441	3.06554301E-02	5.83174678E-01
442	3.04414953E-02	5.83174678E-01
443	3.02287927E-02	5.83174678E-01
444	3.00173191E-02	5.83174678E-01
445	2.98070710E-02	5.83174678E-01
446	2.95980450E-02	5.83174678E-01
447	2.93902376E-02	5.83174678E-01
448	2.91836452E-02	5.83174678E-01
449	2.89782643E-02	5.83174678E-01
450	2.87740911E-02	5.83174678E-01

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GOLD

VALUES FOR PSI(R) AND PSI(R) PSI(R)*. R IN UNITS OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666 RYDBERGS.

R	PSI(R)	PSI(R)PSI(R)*
451	2.85711219E-02	5.83174678E-01
452	2.83693530E-02	5.83174678E-01
453	2.81687805E-02	5.83174678E-01
454	2.79694005E-02	5.83174678E-01
455	2.77712093E-02	5.83174678E-01
456	2.75742027E-02	5.83174678E-01
457	2.73785768E-02	5.83174678E-01
458	2.71837275E-02	5.83174678E-01
459	2.69902508E-02	5.83174678E-01
460	2.67979425E-02	5.83174678E-01
461	2.66067985E-02	5.83174678E-01
462	2.64168146E-02	5.83174678E-01
463	2.62279865E-02	5.83174678E-01
464	2.60403100E-02	5.83174678E-01
465	2.58537807E-02	5.83174678E-01
466	2.56683944E-02	5.83174678E-01
467	2.54841467E-02	5.83174678E-01
468	2.53010331E-02	5.83174678E-01
469	2.51190492E-02	5.83174678E-01
470	2.49381906E-02	5.83174678E-01
471	2.47584529E-02	5.83174678E-01
472	2.45798314E-02	5.83174678E-01
473	2.44023218E-02	5.83174678E-01
474	2.42259193E-02	5.83174678E-01
475	2.40506195E-02	5.83174678E-01
476	2.38764177E-02	5.83174678E-01
477	2.37033094E-02	5.83174678E-01
478	2.35312899E-02	5.83174678E-01
479	2.33603545E-02	5.83174678E-01
480	2.31904985E-02	5.83174678E-01
481	2.30217174E-02	5.83174678E-01
482	2.28540067E-02	5.83174678E-01
483	2.26873605E-02	5.83174678E-01
484	2.25217753E-02	5.83174678E-01
485	2.23572459E-02	5.83174678E-01
486	2.21937676E-02	5.83174678E-01
487	2.20313357E-02	5.83174678E-01
488	2.18699452E-02	5.83174678E-01
489	2.17095914E-02	5.83174678E-01
490	2.15502696E-02	5.83174678E-01
491	2.13919748E-02	5.83174678E-01
492	2.12347022E-02	5.83174678E-01
493	2.10784471E-02	5.83174678E-01
494	2.09232045E-02	5.83174678E-01
495	2.07689697E-02	5.83174678E-01
496	2.06157377E-02	5.83174678E-01
497	2.04635037E-02	5.83174678E-01
498	2.03122628E-02	5.83174678E-01
499	2.01620103E-02	5.83174678E-01
500	2.00127410E-02	5.83174678E-01

TABLE VI

GOLD

VALUES FOR PSI(R) AND PSI(R) PSI(R)*. R IN UNITS OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666 RYDBERGS.

R	PSI(R)	PSI(R)PSI(R)*
501	1.98644504E-02	5.83174678E-01
502	1.97171333E-02	5.83174678E-01
503	1.95707850E-02	5.83174678E-01
504	1.94254006E-02	5.83174678E-01
505	1.92809751E-02	5.83174678E-01
506	1.91375038E-02	5.83174678E-01
507	1.89949816E-02	5.83174678E-01
508	1.88534039E-02	5.83174678E-01
509	1.87127656E-02	5.83174678E-01
510	1.85730618E-02	5.83174678E-01
511	1.84342878E-02	5.83174678E-01
512	1.82964386E-02	5.83174678E-01
513	1.81595094E-02	5.83174678E-01
514	1.80234953E-02	5.83174678E-01
515	1.78883914E-02	5.83174678E-01
516	1.77541929E-02	5.83174678E-01
517	1.76208950E-02	5.83174678E-01
518	1.74884927E-02	5.83174678E-01
519	1.73569812E-02	5.83174678E-01
520	1.72263558E-02	5.83174678E-01
521	1.70966116E-02	5.83174678E-01
522	1.69677457E-02	5.83174678E-01
523	1.68397473E-02	5.83174678E-01
524	1.67126177E-02	5.83174678E-01
525	1.65863501E-02	5.83174678E-01
526	1.64609395E-02	5.83174678E-01
527	1.63363814E-02	5.83174678E-01
528	1.62126708E-02	5.83174678E-01
529	1.60898031E-02	5.83174678E-01
530	1.59677735E-02	5.83174678E-01
531	1.58465772E-02	5.83174678E-01
532	1.57262095E-02	5.83174678E-01
533	1.56066657E-02	5.83174678E-01
534	1.54879411E-02	5.83174678E-01
535	1.53700310E-02	5.83174678E-01
536	1.52529306E-02	5.83174678E-01
537	1.51366353E-02	5.83174678E-01
538	1.50211405E-02	5.83174678E-01
539	1.49064414E-02	5.83174678E-01
540	1.47925335E-02	5.83174678E-01
541	1.46794121E-02	5.83174678E-01
542	1.45670727E-02	5.83174678E-01
543	1.44555105E-02	5.83174678E-01
544	1.43447210E-02	5.83174678E-01
545	1.42346996E-02	5.83174678E-01
546	1.41254410E-02	5.83174678E-01
547	1.40169430E-02	5.83174678E-01
548	1.39091987E-02	5.83174678E-01
549	1.38022043E-02	5.83174678E-01
550	1.36959554E-02	5.83174678E-01

TABLE VI

GOLD

VALUES FOR PSI(R) AND PSI(R) PSI(R)*. R IN UNITS OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666 RYDBERGS.

R	PSI(R)	PSI(R)PSI(R)*
551	1.35904475E-02	5.83174678E-01
552	1.34856760E-02	5.83174678E-01
553	1.33816366E-02	5.83174678E-01
554	1.32783247E-02	5.83174678E-01
555	1.31757360E-02	5.83174678E-01
556	1.30738660E-02	5.83174678E-01
557	1.29727103E-02	5.83174678E-01
558	1.28722645E-02	5.83174678E-01
559	1.27725243E-02	5.83174678E-01
560	1.26734953E-02	5.83174678E-01
561	1.25751432E-02	5.83174678E-01
562	1.24774936E-02	5.83174678E-01
563	1.23805322E-02	5.83174678E-01
564	1.22842548E-02	5.83174678E-01
565	1.21886571E-02	5.83174678E-01
566	1.20937347E-02	5.83174678E-01
567	1.19994836E-02	5.83174678E-01
568	1.19058924E-02	5.83174678E-01
569	1.18129779E-02	5.83174678E-01
570	1.17207130E-02	5.83174678E-01
571	1.16291065E-02	5.83174678E-01
572	1.15381432E-02	5.83174678E-01
573	1.14478359E-02	5.83174678E-01
574	1.13581657E-02	5.83174678E-01
575	1.12691333E-02	5.83174678E-01
576	1.11807346E-02	5.83174678E-01
577	1.109296[illegible]-02	5.83174678E-01
578	1.100582[illegible]-02	5.83174678E-01
579	1.091930[illegible]7E-02	5.83174678E-01
580	1.08333966E-02	5.83174678E-01
581	1.07481061E-02	5.83174678E-01
582	1.06634252E-02	5.83174678E-01
583	1.05793499E-02	5.83174678E-01
584	1.04958764E-02	5.83174678E-01
585	1.04130006E-02	5.83174678E-01
586	1.03307137E-02	5.83174678E-01
587	1.02490269E-02	5.83174678E-01
588	1.01679209E-02	5.83174678E-01
589	1.0087597[illegible]E-02	5.83174678E-01
590	1.00074521E-02	5.83174678E-01
591	9.92808143E-03	5.83174678E-01
592	9.84928136E-03	5.83174678E-01
593	9.77104867E-03	5.83174678E-01
594	9.69337901E-03	5.83174678E-01
595	9.61626932E-03	5.83174678E-01
596	9.53971436E-03	5.83174678E-01
597	9.46371193E-03	5.83174678E-01
598	9.38825784E-03	5.83174678E-01
599	9.31334840E-03	5.83174678E-01
600	9.23897996E-03	5.83174678E-01

TABLE VI

GOLD

VALUES FOR PSI(R) AND PSI(R) PSI(R)*. R IN UNITS OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666 RYDBERGS.

R	PSI(R)	PSI(R)PSI(R)*
601	9.16514887E-03	5.83174678E-01
602	9.09185152E-03	5.83174678E-01
603	9.01908430E-03	5.83174678E-01
604	8.94684362E-03	5.83174678E-01
605	8.87512591E-03	5.83174678E-01
606	8.80392764E-03	5.83174678E-01
607	8.73324525E-03	5.83174678E-01
608	8.66307525E-03	5.83174678E-01
609	8.59341413E-03	5.83174678E-01
610	8.52425842E-03	5.83174678E-01
611	8.45560465E-03	5.83174678E-01
612	8.38744939E-03	5.83174678E-01
613	8.31978921E-03	5.83174678E-01
614	8.25262071E-03	5.83174678E-01
615	8.18594049E-03	5.83174678E-01
616	8.11974519E-03	5.83174678E-01
617	8.05403146E-03	5.83174678E-01
618	7.98879596E-03	5.83174678E-01
619	7.92403537E-03	5.83174678E-01
620	7.85974639E-03	5.83174678E-01
621	7.79592575E-03	5.83174678E-01
622	7.73257019E-03	5.83174678E-01
623	7.66967645E-03	5.83174678E-01
624	7.60724130E-03	5.83174678E-01
625	7.54526155E-03	5.83174678E-01
626	7.48373399E-03	5.83174678E-01
627	7.42265545E-03	5.83174678E-01
628	7.36202277E-03	5.83174678E-01
629	7.30183282E-03	5.83174678E-01
630	7.24208247E-03	5.83174678E-01
631	7.18276861E-03	5.83174678E-01
632	7.12388816E-03	5.83174678E-01
633	7.06543904E-03	5.83174678E-01
634	7.00741520E-03	5.83174678E-01
635	6.94981662E-03	5.83174678E-01
636	6.89263925E-03	5.83174678E-01
637	6.83588012E-03	5.83174678E-01
638	6.77953622E-03	5.83174678E-01
639	6.72360460E-03	5.83174678E-01
640	6.66808229E-03	5.83174678E-01
641	6.61296637E-03	5.83174678E-01
642	6.55825392E-03	5.83174678E-01
643	6.50394204E-03	5.83174678E-01
644	6.45002775E-03	5.83174678E-01
645	6.39650847E-03	5.83174678E-01
646	6.34338106E-03	5.83174678E-01
647	6.29064278E-03	5.83174678E-01
648	6.23829082E-03	5.83174678E-01
649	6.18632238E-03	5.83174678E-01
650	6.13473466E-03	5.83174678E-01

TABLE VI

GOLD

VALUES FOR PSI(R) AND PSI(R) PSI(R)*. R IN UNITS OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666 RYDBERGS.

R	PSI(R)	PSI(R)PSI(R)*
651	6.08352491E-03	5.83174678E-01
652	6.03269017E-03	5.83174678E-01
653	5.98222752E-03	5.83174678E-01
654	5.93213406E-03	5.83174678E-01
655	5.88240639E-03	5.83174678E-01
656	5.83304316E-03	5.83174678E-01
657	5.78404003E-03	5.83174678E-01
658	5.73539467E-03	5.83174678E-01
659	5.68710427E-03	5.83174678E-01
660	5.63916606E-03	5.83174678E-01
661	5.59157727E-03	5.83174678E-01
662	5.54433517E-03	5.83174678E-01
663	5.49743701E-03	5.83174678E-01
664	5.45088011E-03	5.83174678E-01
665	5.40466178E-03	5.83174678E-01
666	5.35877935E-03	5.83174678E-01
667	5.31323017E-03	5.83174678E-01
668	5.26801162E-03	5.83174678E-01
669	5.22312109E-03	5.83174678E-01
670	5.17855599E-03	5.83174678E-01
671	5.13431374E-03	5.83174678E-01
672	5.09039190E-03	5.83174678E-01
673	5.04678763E-03	5.83174678E-01
674	5.00349370E-03	5.83174678E-01
675	4.96052253E-03	5.83174678E-01
676	4.91785662E-03	5.83174678E-01
677	4.87549852E-03	5.83174678E-01
678	4.83344578E-03	5.83174678E-01
679	4.79169597E-03	5.83174678E-01
680	4.75024668E-03	5.83174678E-01
681	4.70909552E-03	5.83174678E-01
682	4.66824010E-03	5.83174678E-01
683	4.62767307E-03	5.83174678E-01
684	4.58740708E-03	5.83174678E-01
685	4.54742430E-03	5.83174678E-01
686	4.50772394E-03	5.83174678E-01
687	4.46831718E-03	5.83174678E-01
688	4.42918726E-03	5.83174678E-01
689	4.39033691E-03	5.83174678E-01
690	4.35176398E-03	5.83174678E-01
691	4.31346595E-03	5.83174678E-01
692	4.27544091E-03	5.83174678E-01
693	4.23768654E-03	5.83174678E-01
694	4.20020068E-03	5.83174678E-01
695	4.16298116E-03	5.83174678E-01
696	4.12602582E-03	5.83174678E-01
697	4.08933252E-03	5.83174678E-01
698	4.05289915E-03	5.83174678E-01
699	4.01672360E-03	5.83174678E-01
700	3.98080378E-03	5.83174678E-01

TABLE VI

GOLD

VALUES FOR PSI(R) AND PSI(R) PSI(R)*. R IN UNITS OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666 RYDBERGS.

R	PSI(R)	PSI(R)PSI(R)*
701	3.94513760E-03	5.83174678E-01
702	3.90972301E-03	5.83174678E-01
703	3.87455797E-03	5.83174678E-01
704	3.83964043E-03	5.83174678E-01
705	3.80496837E-03	5.83174678E-01
706	3.77053981E-03	5.83174678E-01
707	3.73635273E-03	5.83174678E-01
708	3.70240517E-03	5.83174678E-01
709	3.66869517E-03	5.83174678E-01
710	3.63522077E-03	5.83174678E-01
711	3.60198004E-03	5.83174678E-01
712	3.56897106E-03	5.83174678E-01
713	3.53619192E-03	5.83174678E-01
714	3.50364072E-03	5.83174678E-01
715	3.47131559E-03	5.83174678E-01
716	3.43921466E-03	5.83174678E-01
717	3.40733607E-03	5.83174678E-01
718	3.37567798E-03	5.83174678E-01
719	3.34403855E-03	5.83174678E-01
720	3.31301597E-03	5.83174678E-01
721	3.28200946E-03	5.83174678E-01
722	3.25121420E-03	5.83174678E-01
723	3.22063141E-03	5.83174678E-01
724	3.19025934E-03	5.83174678E-01
725	3.16009323E-03	5.83174678E-01
726	3.13013434E-03	5.83174678E-01
727	3.10037993E-03	5.83174678E-01
728	3.07082829E-03	5.83174678E-01
729	3.04147772E-03	5.83174678E-01
730	3.01232651E-03	5.83174678E-01
731	2.98337299E-03	5.83174678E-01
732	2.95461549E-03	5.83174678E-01
733	2.92605235E-03	5.83174678E-01
734	2.89768191E-03	5.83174678E-01
735	2.86950255E-03	5.83174678E-01
736	2.84151263E-03	5.83174678E-01
737	2.81371055E-03	5.83174678E-01
738	2.78609470E-03	5.83174678E-01
739	2.75866349E-03	5.83174678E-01
740	2.73141534E-03	5.83174678E-01
741	2.70434868E-03	5.83174678E-01
742	2.67746195E-03	5.83174678E-01
743	2.65075359E-03	5.83174678E-01
744	2.62422208E-03	5.83174678E-01
745	2.59786589E-03	5.83174678E-01
746	2.57168349E-03	5.83174678E-01
747	2.54567339E-03	5.83174678E-01
748	2.51983408E-03	5.83174678E-01
749	2.49416408E-03	5.83174678E-01
750	2.46866191E-03	5.83174678E-01

TABLE VI

GOLD

VALUES FOR PSI(R) AND PSI(R) PSI(R)*. R IN UNITS OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666 RYDBERGS.

R	PSI(R)	PSI(R)PSI(R)*
751	2.44332611E-03	5.83174678E-01
752	2.41815521E-03	5.83174678E-01
753	2.39314778E-03	5.83174678E-01
754	2.36830238E-03	5.83174678E-01
755	2.34361757E-03	5.83174678E-01
756	2.31909195E-03	5.83174678E-01
757	2.29472410E-03	5.83174678E-01
758	2.27051262E-03	5.83174678E-01
759	2.24645613E-03	5.83174678E-01
760	2.22255325E-03	5.83174678E-01
761	2.19880261E-03	5.83174678E-01
762	2.17520293E-03	5.83174678E-01
763	2.15175258E-03	5.83174678E-01
764	2.12845051E-03	5.83174678E-01
765	2.10529529E-03	5.83174678E-01
766	2.08228559E-03	5.83174678E-01
767	2.05942027E-03	5.83174678E-01
768	2.03669746E-03	5.83174678E-01
769	2.01411644E-03	5.83174678E-01
770	1.99167573E-03	5.83174678E-01
771	1.96937403E-03	5.83174678E-01
772	1.94721007E-03	5.83174678E-01
773	1.92518261E-03	5.83174678E-01
774	1.90329037E-03	5.83174678E-01
775	1.88153210E-03	5.83174678E-01
776	1.85990657E-03	5.83174678E-01
777	1.83841253E-03	5.83174678E-01
778	1.81704877E-03	5.83174678E-01
779	1.79581407E-03	5.83174678E-01
780	1.77470722E-03	5.83174678E-01
781	1.75372702E-03	5.83174678E-01
782	1.73287227E-03	5.83174678E-01
783	1.71214179E-03	5.83174678E-01
784	1.69153440E-03	5.83174678E-01
785	1.67104892E-03	5.83174678E-01
786	1.65068421E-03	5.83174678E-01
787	1.63043909E-03	5.83174678E-01
788	1.61031243E-03	5.83174678E-01
789	1.59030307E-03	5.83174678E-01
790	1.57040989E-03	5.83174678E-01
791	1.55063176E-03	5.83174678E-01
792	1.53096756E-03	5.83174678E-01
793	1.51141618E-03	5.83174678E-01
794	1.49197650E-03	5.83174678E-01
795	1.47264744E-03	5.83174678E-01
796	1.45342790E-03	5.83174678E-01
797	1.43431679E-03	5.83174678E-01
798	1.41531304E-03	5.83174678E-01
799	1.39641557E-03	5.83174678E-01
800	1.37762331E-03	5.83174678E-01

```
                    TABLE VI

                      GOLD

     VALUES FOR PSI(R) AND PSI(R) PSI(R)*. R IN UNITS
     OF 1/100 BOHR UNITS. IONIZATION ENERGY IS .666
     RYDBERGS.

      R                 PSI(R)                    PSI(R)PSI(R)*


    801            1.35893522E-03             5.83174678E-01
    802            1.34035024E-03             5.83174678E-01
    803            1.32186731E-03             5.83174678E-01
    804            1.30348541E-03             5.83174678E-01
    805            1.28520350E-03             5.83174678E-01
    806            1.26700055E-03             5.83174678E-01
    807            1.24893554E-03             5.83174678E-01
    808            1.23094746E-03             5.83174678E-01
    809            1.21305529E-03             5.83174678E-01
    810            1.19525804E-03             5.83174678E-01
    811            1.17755472E-03             5.83174678E-01
    812            1.15994432E-03             5.83174678E-01
    813            1.14242586E-03             5.83174678E-01
    814            1.12499837E-03             5.83174678E-01
    815            1.10766087E-03             5.83174678E-01
    816            1.09041240E-03             5.83174678E-01
    817            1.07325199E-03             5.83174678E-01
    818            1.05617869E-03             5.83174678E-01
    819            1.03919155E-03             5.83174678E-01
    820            1.02228961E-03             5.83174678E-01
    821            1.0054710[illegible]E-03             5.83174678E-01
    822            9.887676[illegible]E-04             5.83174678E-01
    823            9.7208573[illegible]E-04             5.83174678E-01
    824            9.55152866E-04             5.83174678E-01
    825            9.39025424E-04             5.83174678E-01
    826            9.22615216E-04             5.83174678E-01
    827            9.06283753E-04             5.83174678E-01
    828            8.90030133E-04             5.83174678E-01
    829            8.73857458E-04             5.83174678E-01
    830            8.57752835E-04             5.83174678E-01
TIME,  1 MINUTES AND   2 SECONDS
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TABLE VII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
1	7.63668275E-03	7.63668275E-01
2	2.80575038E-02	1.40287519E+00
3	2.97277998E-02	9.90926660E-01
4	1.86657869E-02	4.66644673E-01
5	1.80550235E-03	3.61100469E-02
6	-1.54903306E-02	-2.58172176E-01
7	-2.97551698E-02	-4.25073854E-01
8	-3.91526554E-02	-4.89408193E-01
9	-4.30755542E-02	-4.78617269E-01
10	-4.17613816E-02	-4.17613816E-01
11	-3.59724647E-02	-3.27022406E-01
12	-2.67490334E-02	-2.22908612E-01
13	-1.52291669E-02	-1.17147438E-01
14	-2.52462309E-03	-1.80330221E-02
15	1.03590390E-02	6.90602598E-02
16	2.25685805E-02	1.41053628E-01
17	3.34243650E-02	1.96613912E-01
18	4.24240319E-02	2.35689066E-01
19	4.92342486E-02	2.59127624E-01
20	5.36749065E-02	2.68374532E-01
21	5.56990276E-02	2.65233465E-01
22	5.53707721E-02	2.51685328E-01
23	5.28432372E-02	2.29753205E-01
24	4.83372020E-02	2.01405009E-01
25	4.21215589E-02	1.68486236E-01
26	3.44958656E-02	1.32676406E-01
27	2.57752255E-02	9.54637980E-02
28	1.62775400E-02	5.81340716E-02
29	6.31306601E-03	2.17691932E-02
30	-3.82386553E-03	-1.27462184E-02
31	-1.38611567E-02	-4.47134088E-02
32	-2.35534908E-02	-7.36046587E-02
33	-3.26853428E-02	-9.90464935E-02
34	-4.10726750E-02	-1.20801985E-01
35	-4.85635272E-02	-1.38752935E-01
36	-5.50377017E-02	-1.52882505E-01
37	-6.04057212E-02	-1.63258706E-01
38	-6.46072234E-02	-1.70019009E-01
39	-6.76089328E-02	-1.73356238E-01
40	-6.94023367E-02	-1.73505842E-01
41	-7.00011679E-02	-1.70734556E-01
42	-6.94387872E-02	-1.65330446E-01
43	-6.77655374E-02	-1.57594273E-01
44	-6.50461299E-02	-1.47832113E-01
45	-6.13571126E-02	-1.36349139E-01
46	-5.67844555E-02	-1.23444469E-01
47	-5.14212821E-02	-1.09406983E-01
48	-4.53657666E-02	-9.45120138E-02
49	-3.87192099E-02	-7.90187957E-02
50	-3.15843003E-02	-6.31686006E-02

TABLE VII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
51	-2.40635632E-02	-4.71834572E-02
52	-1.62579963E-02	-3.12653776E-02
53	-8.26588762E-03	-1.55960144E-02
54	-1.81806782E-04	-3.36679225E-04
55	7.90423651E-03	1.43713391E-02
56	1.59074793E-02	2.84062130E-02
57	2.37489474E-02	4.16648199E-02
58	3.13558647E-02	5.40618357E-02
59	3.86619419E-02	6.55287150E-02
60	4.56075555E-02	7.60125925E-02
61	5.21398307E-02	8.54751323E-02
62	5.82126372E-02	9.38913503E-02
63	6.37865110E-02	1.01248430E-01
64	6.88285110E-02	1.07544548E-01
65	7.33120207E-02	1.12787724E-01
66	7.72165040E-02	1.16994703E-01
67	8.05272240E-02	1.20189887E-01
68	8.32349306E-02	1.22404310E-01
69	8.53355268E-02	1.23674676E-01
70	8.68297169E-02	1.24042453E-01
71	8.77226449E-02	1.23553021E-01
72	8.80235259E-02	1.22254897E-01
73	8.77452762E-02	1.20199008E-01
74	8.69041468E-02	1.17438036E-01
75	8.55193603E-02	1.14025914E-01
76	8.36127579E-02	1.10016787E-01
77	8.12084566E-02	1.05465528E-01
78	7.83325199E-02	1.00426306E-01
79	7.50126373E-02	9.49527055E-02
80	7.12778342E-02	8.90972928E-02
81	6.71581779E-02	8.29113307E-02
82	6.26845160E-02	7.64445317E-02
83	5.78882270E-02	6.97448518E-02
84	5.28009385E-02	6.28583196E-02
85	4.74545642E-02	5.58288991E-02
86	4.18806081E-02	4.86983815E-02
87	3.61104861E-02	4.15063058E-02
88	3.01751147E-02	3.42899031E-02
89	2.41043162E-02	2.70840632E-02
90	1.79291898E-02	1.99213220E-02
91	1.16769975E-02	1.28318654E-02
92	5.37606551E-03	5.84334947E-03
93	-9.46801277E-04	-1.01806589E-03
94	-7.26589159E-03	-7.72967191E-03
95	-1.35566476E-02	-1.42701553E-02
96	-1.97957131E-02	-2.06205345E-02
97	-2.59609717E-02	-2.67638883E-02
98	-3.20315738E-02	-3.26852793E-02
99	-3.79879556E-02	-3.83716724E-02
100	-4.38118491E-02	-4.38118491E-02

TABLE VII

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LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
101	-4.94862342E-02	-4.89963210E-02
102	-5.49955839E-02	-5.39172391E-02
103	-6.03253537E-02	-5.85683046E-02
104	-6.54624646E-02	-6.29446775E-02
105	-7.03950312E-02	-6.70428869E-02
106	-7.51123356E-02	-7.08607411E-02
107	-7.96050469E-02	-7.43972401E-02
108	-8.38646879E-02	-7.76524888E-02
109	-8.78840982E-02	-8.06276130E-02
110	-9.16571455E-02	-8.33246777E-02
111	-9.51787342E-02	-8.57466074E-02
112	-9.84447631E-02	-8.78971099E-02
113	-1.01452081E-01	-8.97806025E-02
114	-1.04199442E-01	-9.14021417E-02
115	-1.06682459E-01	-9.27673559E-02
116	-1.08903562E-01	-9.38823808E-02
117	-1.10861945E-01	-9.47537990E-02
118	-1.12558526E-01	-9.53885816E-02
119	-1.13994901E-01	-9.57940342E-02
120	-1.15173295E-01	-9.59777454E-02
121	-1.16096522E-01	-9.59475385E-02
122	-1.16767940E-01	-9.57114262E-02
123	-1.17191410E-01	-9.51775687E-02
124	-1.17371251E-01	-9.46542344E-02
125	-1.17312204E-01	-9.38497634E-02
126	-1.17019392E-01	-9.28725337E-02
127	-1.16498282E-01	-9.17309303E-02
128	-1.15754646E-01	-9.04333169E-02
129	-1.14794532E-01	-8.89880092E-02
130	-1.13624227E-01	-8.74032518E-02
131	-1.12250227E-01	-8.56871960E-02
132	-1.10679203E-01	-8.39478809E-02
133	-1.08917977E-01	-8.18932156E-02
134	-1.06973491E-01	-7.98309636E-02
135	-1.04852724E-01	-7.76687291E-02
136	-1.02562965E-01	-7.54139449E-02
137	-1.00111190E-01	-7.30738616E-02
138	-9.75046439E-02	-7.06555390E-02
139	-9.47505148E-02	-6.81658380E-02
140	-9.18559798E-02	-6.56114141E-02
141	-8.88281851E-02	-6.29987128E-02
142	-8.56742301E-02	-6.03339648E-02
143	-8.24011524E-02	-5.76231835E-02
144	-7.90159141E-02	-5.48721626E-02
145	-7.55253985E-02	-5.20864748E-02
146	-7.19363490E-02	-4.92714719E-02
147	-6.82554581E-02	-4.64322844E-02
148	-6.44892582E-02	-4.35738231E-02
149	-6.06441627E-02	-4.07007803E-02
150	-5.67264484E-02	-3.78176323E-02

TABLE VII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
151	-5.27422438E-02	-3.49286416E-02
152	-4.86975479E-02	-3.20378605E-02
153	-4.45981753E-02	-2.91491342E-02
154	-4.04498017E-02	-2.62661050E-02
155	-3.62579348E-02	-2.33922160E-02
156	-3.20279170E-02	-2.05307160E-02
157	-2.77649222E-02	-1.76846639E-02
158	-2.34739546E-02	-1.48569333E-02
159	-1.91598467E-02	-1.20502181E-02
160	-1.48272594E-02	-9.26703711E-03
161	-1.04806808E-02	-6.50973965E-03
162	-6.12442718E-03	-3.78051061E-03
163	-1.76264280E-03	-1.08137595E-03
164	2.60069864E-03	1.58579185E-03
165	6.96179293E-03	4.21926844E-03
166	1.13170073E-02	6.81747214E-03
167	1.56628607E-02	9.37895852E-03
168	1.99960573E-02	1.19024151E-02
169	2.43134483E-02	1.43866558E-02
170	2.86120474E-02	1.68306161E-02
171	3.28890242E-02	1.92333475E-02
172	3.71417013E-02	2.15940124E-02
173	4.13675511E-02	2.39113793E-02
174	4.55641929E-02	2.61863177E-02
175	4.97293887E-02	2.84167935E-02
176	5.38610406E-02	3.06028640E-02
177	5.79571867E-02	3.27441733E-02
178	6.20159976E-02	3.48404481E-02
179	6.60357728E-02	3.68914932E-02
180	7.00149369E-02	3.88971871E-02
181	7.39520354E-02	4.08574781E-02
182	7.78457322E-02	4.27723903E-02
183	8.16948041E-02	4.46419695E-02
184	8.54981334E-02	4.64663796E-02
185	8.92547284E-02	4.82457991E-02
186	9.29636699E-02	4.99804677E-02
187	9.66241574E-02	5.16706724E-02
188	1.00235430E-01	5.33167449E-02
189	1.03797020E-01	5.49190582E-02
190	1.07308245E-01	5.64780234E-02
191	1.10769707E-01	5.79940875E-02
192	1.14178041E-01	5.94677298E-02
193	1.17535958E-01	6.08994600E-02
194	1.20842241E-01	6.22898151E-02
195	1.24096747E-01	6.36393576E-02
196	1.27299398E-01	6.49486726E-02
197	1.30450181E-01	6.62183659E-02
198	1.33549143E-01	6.74490621E-02
199	1.36596390E-01	6.86414020E-02
200	1.39592083E-01	6.97960415E-02

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LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
201	1.42536435E-01	7.09136493E-02
202	1.45429708E-01	7.19942051E-02
203	1.48272212E-01	7.30404984E-02
204	1.51064298E-01	7.40511266E-02
205	1.53806363E-01	7.50274940E-02
206	1.56498838E-01	7.59703099E-02
207	1.59142195E-01	7.68802874E-02
208	1.61736937E-01	7.77581428E-02
209	1.64283601E-01	7.86045937E-02
210	1.66782752E-01	7.94203582E-02
211	1.69234935E-01	8.02061540E-02
212	1.71640919E-01	8.09626975E-02
213	1.74001196E-01	8.16907025E-02
214	1.76316483E-01	8.23908801E-02
215	1.78587465E-01	8.30639372E-02
216	1.80814844E-01	8.37105760E-02
217	1.82999342E-01	8.43314939E-02
218	1.85141693E-01	8.49273819E-02
219	1.87242646E-01	8.54989250E-02
220	1.89302962E-01	8.60468010E-02
221	1.91323413E-01	8.65716802E-02
222	1.93304780E-01	8.70742253E-02
223	1.95247850E-01	8.75550905E-02
224	1.97153424E-01	8.80149215E-02
225	1.99022299E-01	8.84543550E-02
226	2.00855282E-01	8.88740184E-02
227	2.02653182E-01	8.92745296E-02
228	2.04416813E-01	8.96564968E-02
229	2.06146987E-01	9.00205183E-02
230	2.07844519E-01	9.03671822E-02
231	2.09510223E-01	9.06970662E-02
232	2.11144912E-01	9.10107378E-02
233	2.12749397E-01	9.13087539E-02
234	2.14324486E-01	9.15916608E-02
235	2.15870986E-01	9.18599939E-02
236	2.17389627E-01	9.21142784E-02
237	2.18881417E-01	9.23550281E-02
238	2.20346937E-01	9.25827466E-02
239	2.21787044E-01	9.27979264E-02
240	2.23202518E-01	9.30010493E-02
241	2.24594133E-01	9.31925865E-02
242	2.25962656E-01	9.33729982E-02
243	2.27308845E-01	9.35427344E-02
244	2.28633451E-01	9.37022342E-02
245	2.29937219E-01	9.38519262E-02
246	2.31220933E-01	9.39922288E-02
247	2.32485168E-01	9.41235497E-02
248	2.33730791E-01	9.42462868E-02
249	2.34958460E-01	9.43608274E-02
250	2.36168873E-01	9.44675490E-02

TABLE VII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
251	2.37362717E-01	9.45668193E-02
252	2.38540670E-01	9.46589960E-02
253	2.39707400E-01	9.47444270E-02
254	2.40851566E-01	9.48234510E-02
255	2.41985812E-01	9.48963970E-02
256	2.43106777E-01	9.49635849E-02
257	2.44215036E-01	9.50253252E-02
258	2.45311353E-01	9.50819196E-02
259	2.46396182E-01	9.51336610E-02
260	2.47470166E-01	9.51808333E-02
261	2.48533988E-01	9.52237119E-02
262	2.49587918E-01	9.52625641E-02
263	2.50632815E-01	9.52976484E-02
264	2.51669129E-01	9.53292155E-02
265	2.52697396E-01	9.53575080E-02
266	2.53718143E-01	9.53827607E-02
267	2.54731886E-01	9.54052006E-02
268	2.55739127E-01	9.54250473E-02
269	2.56740359E-01	9.54425128E-02
270	2.57736066E-01	9.54578020E-02
271	2.58726716E-01	9.54711127E-02
272	2.59712769E-01	9.54826357E-02
273	2.60694674E-01	9.54925547E-02
274	2.61672869E-01	9.55010472E-02
275	2.62647730E-01	9.55082838E-02
276	2.63619824E-01	9.55144283E-02
277	2.64589403E-01	9.55196402E-02
278	2.65556915E-01	9.55240700E-02
279	2.66522740E-01	9.55278640E-02
280	2.67487254E-01	9.55311621E-02
281	2.68450818E-01	9.55340988E-02
282	2.69413734E-01	9.55368027E-02
283	2.70376493E-01	9.55393969E-02
284	2.71339278E-01	9.55419992E-02
285	2.72302458E-01	9.55447222E-02
286	2.73266346E-01	9.55476734E-02
287	2.74231241E-01	9.55509552E-02
288	2.75197435E-01	9.55546651E-02
289	2.76165209E-01	9.55588960E-02
290	2.77134834E-01	9.55637359E-02
291	2.78106571E-01	9.55692684E-02
292	2.79080672E-01	9.55755707E-02
293	2.80057330E-01	9.55827235E-02
294	2.81036926E-01	9.55907913E-02
295	2.82019536E-01	9.55998425E-02
296	2.83005421E-01	9.56099396E-02
297	2.83994738E-01	9.56211409E-02
298	2.84987333E-01	9.56335010E-02
299	2.85984741E-01	9.56470706E-02
300	2.86985691E-01	9.56618970E-02

TABLE VII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
301	2.87990728E-01	9.56779827E-02
302	2.89000016E-01	9.56953696E-02
303	2.90013720E-01	9.57140991E-02
304	2.91032005E-01	9.57342123E-02
305	2.92055035E-01	9.57557492E-02
306	2.93082975E-01	9.57787490E-02
307	2.94115998E-01	9.58032536E-02
308	2.95154241E-01	9.58292990E-02
309	2.96197896E-01	9.58569243E-02
310	2.97247119E-01	9.58861675E-02
311	2.98302074E-01	9.59170657E-02
312	2.99362926E-01	9.59496559E-02
313	3.00429840E-01	9.59839744E-02
314	3.01502980E-01	9.60200572E-02
315	3.02582510E-01	9.60579398E-02
316	3.03668597E-01	9.60976572E-02
317	3.04761404E-01	9.61392443E-02
318	3.05861098E-01	9.61827352E-02
319	3.06967843E-01	9.62281638E-02
320	3.08081804E-01	9.62755638E-02
321	3.09203148E-01	9.63249681E-02
322	3.10332039E-01	9.63764097E-02
323	3.11468644E-01	9.64299209E-02
324	3.12613130E-01	9.64855338E-02
325	3.13765661E-01	9.65432803E-02
326	3.14926405E-01	9.66031916E-02
327	3.16095528E-01	9.66652991E-02
328	3.17273198E-01	9.67296335E-02
329	3.18459581E-01	9.67962253E-02
330	3.19654846E-01	9.68651047E-02
331	3.20859139E-01	9.69363018E-02
332	3.22072690E-01	9.70098463E-02
333	3.23295606E-01	9.70857675E-02
334	3.24528076E-01	9.71640947E-02
335	3.25770270E-01	9.72449568E-02
336	3.27022357E-01	9.73280825E-02
337	3.28284507E-01	9.74138002E-02
338	3.29556890E-01	9.75020384E-02
339	3.30839676E-01	9.75928249E-02
340	3.32133038E-01	9.76861876E-02
341	3.33437146E-01	9.77821543E-02
342	3.34752173E-01	9.78807522E-02
343	3.36078220E-01	9.79820088E-02
344	3.37415672E-01	9.80859511E-02
345	3.38764491E-01	9.81926061E-02
346	3.40124922E-01	9.83020005E-02
347	3.41497139E-01	9.84141610E-02
348	3.42881317E-01	9.85291140E-02
349	3.44277632E-01	9.86468859E-02
350	3.45686260E-01	9.87675029E-02

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LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
351	3.47107379E-01	9.88909910E-02
352	3.48541165E-01	9.90173764E-02
353	3.49987797E-01	9.91466847E-02
354	3.51447454E-01	9.92789418E-02
355	3.52920315E-01	9.94141733E-02
356	3.54406561E-01	9.95524049E-02
357	3.55906373E-01	9.96936619E-02
358	3.57419932E-01	9.98379697E-02
359	3.58947420E-01	9.99853538E-02
360	3.60489021E-01	1.00135839E-01
361	3.62044920E-01	1.00289451E-01
362	3.63615300E-01	1.00446215E-01
363	3.65200347E-01	1.00606156E-01
364	3.66800249E-01	1.00769299E-01
365	3.68415191E-01	1.00935669E-01
366	3.70045364E-01	1.01105291E-01
367	3.71690095E-01	1.01278189E-01
368	3.73352155E-01	1.01454390E-01
369	3.75029154E-01	1.01633917E-01
370	3.76722146E-01	1.01816796E-01
371	3.78431323E-01	1.02003052E-01
372	3.80156878E-01	1.02192709E-01
373	3.81899007E-01	1.02385797E-01
374	3.83657907E-01	1.02582328E-01
375	3.85433773E-01	1.02782739E-01
376	3.87226805E-01	1.02985850E-01
377	3.89037201E-01	1.03192892E-01
378	3.90865163E-01	1.03403402E-01
379	3.92710891E-01	1.03617649E-01
380	3.94574589E-01	1.03835418E-01
381	3.96456461E-01	1.04056214E-01
382	3.98356711E-01	1.04281862E-01
383	4.00275546E-01	1.04510587E-01
384	4.02213175E-01	1.04743014E-01
385	4.04169305E-01	1.04979170E-01
386	4.06145647E-01	1.05219080E-01
387	4.08140913E-01	1.05462768E-01
388	4.10155815E-01	1.05710262E-01
389	4.12190569E-01	1.05961586E-01
390	4.14245389E-01	1.06216766E-01
391	4.16320493E-01	1.06475829E-01
392	4.18416099E-01	1.06738801E-01
393	4.20532428E-01	1.07005707E-01
394	4.22669700E-01	1.07276574E-01
395	4.24828140E-01	1.07551428E-01
396	4.27007970E-01	1.07830296E-01
397	4.29209419E-01	1.08113204E-01
398	4.31432712E-01	1.08400179E-01
399	4.33679080E-01	1.08691248E-01
400	4.35945753E-01	1.08986438E-01

TABLE VII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
401	4.38235964E-01	1.09285777E-01
402	4.40548948E-01	1.09589290E-01
403	4.42884939E-01	1.09897007E-01
404	4.45244176E-01	1.10208955E-01
405	4.47626899E-01	1.10525160E-01
406	4.50033348E-01	1.10845652E-01
407	4.52463766E-01	1.11170458E-01
408	4.54918398E-01	1.11499607E-01
409	4.57397492E-01	1.11833129E-01
410	4.59901295E-01	1.12171047E-01
411	4.62430057E-01	1.12513396E-01
412	4.64984033E-01	1.12860202E-01
413	4.67563475E-01	1.13211495E-01
414	4.70168640E-01	1.13567304E-01
415	4.72799784E-01	1.13927659E-01
416	4.75457175E-01	1.14292590E-01
417	4.78141065E-01	1.14662127E-01
418	4.80851730E-01	1.15036299E-01
419	4.83589427E-01	1.15415138E-01
420	4.86354429E-01	1.15798674E-01
421	4.89147007E-01	1.16186938E-01
422	4.91967434E-01	1.16579961E-01
423	4.94815295E-01	1.16977774E-01
424	4.97692938E-01	1.17380410E-01
425	5.00599574E-01	1.17787900E-01
426	5.03533174E-01	1.18200275E-01
427	5.06497023E-01	1.18617570E-01
428	5.09490409E-01	1.19039815E-01
429	5.12513621E-01	1.19467045E-01
430	5.15566951E-01	1.19899291E-01
431	5.18650694E-01	1.20336588E-01
432	5.21765147E-01	1.20778969E-01
433	5.24910609E-01	1.21226468E-01
434	5.28087382E-01	1.21679120E-01
435	5.31295771E-01	1.22136959E-01
436	5.34536083E-01	1.22600019E-01
437	5.37808629E-01	1.23068336E-01
438	5.41113721E-01	1.23541946E-01
439	5.44451675E-01	1.24020893E-01
440	5.47822809E-01	1.24505184E-01
441	5.51227444E-01	1.24994885E-01
442	5.54665903E-01	1.25490023E-01
443	5.58138514E-01	1.25990635E-01
444	5.61645607E-01	1.26496758E-01
445	5.65187513E-01	1.27008430E-01
446	5.68764568E-01	1.27525688E-01
447	5.72377112E-01	1.28048571E-01
448	5.76025485E-01	1.28577117E-01
449	5.79710033E-01	1.29111366E-01
450	5.83431103E-01	1.29651356E-01

TABLE VII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
451	5.87189045E-01	1.30197128E-01
452	5.90984215E-01	1.30748720E-01
453	5.94816970E-01	1.31306174E-01
454	5.98687670E-01	1.31869531E-01
455	6.02596679E-01	1.32439831E-01
456	6.06544365E-01	1.33014115E-01
457	6.10531098E-01	1.33595426E-01
458	6.14557253E-01	1.34182806E-01
459	6.18623206E-01	1.34776298E-01
460	6.22729339E-01	1.35375943E-01
461	6.26876036E-01	1.35981787E-01
462	6.31063686E-01	1.36593871E-01
463	6.35292631E-01	1.37212242E-01
464	6.39563415E-01	1.37836943E-01
465	6.43876288E-01	1.38468019E-01
466	6.48231702E-01	1.39105516E-01
467	6.52630065E-01	1.39749479E-01
468	6.57071787E-01	1.40399954E-01
469	6.61557232E-01	1.41056990E-01
470	6.66086968E-01	1.41720631E-01
471	6.70661267E-01	1.42390927E-01
472	6.75280606E-01	1.43067925E-01
473	6.79945415E-01	1.43751673E-01
474	6.84656128E-01	1.44442221E-01
475	6.89413183E-01	1.45139618E-01
476	6.94217024E-01	1.45843913E-01
477	6.99068096E-01	1.46555156E-01
478	7.03966352E-01	1.47273400E-01
479	7.08913746E-01	1.47998694E-01
480	7.13909238E-01	1.48731091E-01
481	7.18953792E-01	1.49470643E-01
482	7.24047878E-01	1.50217402E-01
483	7.29191967E-01	1.50971422E-01
484	7.34386538E-01	1.51732756E-01
485	7.39632073E-01	1.52501458E-01
486	7.44929059E-01	1.53277594E-01
487	7.50277927E-01	1.54061188E-01
488	7.55679355E-01	1.54852327E-01
489	7.61133662E-01	1.55651056E-01
490	7.66641416E-01	1.56457432E-01
491	7.72203126E-01	1.57271513E-01
492	7.77819310E-01	1.58093356E-01
493	7.83490488E-01	1.58923020E-01
494	7.89217126E-01	1.59760564E-01
495	7.94999935E-01	1.60606047E-01
496	8.00839271E-01	1.61459530E-01
497	8.06735736E-01	1.62321074E-01
498	8.12689877E-01	1.63190738E-01
499	8.18702246E-01	1.64068586E-01
500	8.24773400E-01	1.64954680E-01

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GOLD

LOWEST ENERGY STATE IS -1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
501	8.30903903E-01	1.65849082E-01
502	8.37094323E-01	1.66751857E-01
503	8.43345235E-01	1.67663069E-01
504	8.49657217E-01	1.68582781E-01
505	8.56030856E-01	1.69511061E-01
506	8.62466743E-01	1.70447973E-01
507	8.68965474E-01	1.71393585E-01
508	8.75527653E-01	1.72347963E-01
509	8.82153889E-01	1.73311177E-01
510	8.88844796E-01	1.74283293E-01
511	8.95600996E-01	1.75264383E-01
512	9.02423115E-01	1.76254515E-01
513	9.09311786E-01	1.77253759E-01
514	9.16267650E-01	1.78262189E-01
515	9.23291352E-01	1.79279874E-01
516	9.30383544E-01	1.80306888E-01
517	9.37544885E-01	1.81343305E-01
518	9.44776040E-01	1.82389197E-01
519	9.52077632E-01	1.83444640E-01
520	9.59450488E-01	1.84509709E-01
521	9.66895144E-01	1.85584481E-01
522	9.74412342E-01	1.86669031E-01
523	9.82002781E-01	1.87763438E-01
524	9.89667166E-01	1.88867780E-01
525	9.97406211E-01	1.89982135E-01
526	1.00522064E+00	1.91106585E-01
527	1.01311117E+00	1.92241208E-01
528	1.02107854E+00	1.93386087E-01
529	1.02912349E+00	1.94541303E-01
530	1.03724678E+00	1.95706940E-01
531	1.04544916E+00	1.96883080E-01
532	1.05373139E+00	1.98069809E-01
533	1.06209424E+00	1.99267212E-01
534	1.07053950E+00	2.00475374E-01
535	1.07906495E+00	2.01694382E-01
536	1.08767438E+00	2.02924325E-01
537	1.09636761E+00	2.04165290E-01
538	1.10514543E+00	2.05417367E-01
539	1.11400868E+00	2.06680646E-01
540	1.12295817E+00	2.07955217E-01
541	1.13199475E+00	2.09241174E-01
542	1.14111926E+00	2.10538608E-01
543	1.15033254E+00	2.11847614E-01
544	1.15963547E+00	2.13168285E-01
545	1.16902891E+00	2.14500717E-01
546	1.17851373E+00	2.15845006E-01
547	1.18809034E+00	2.17201250E-01
548	1.19776112E+00	2.18569547E-01
549	1.20752547E+00	2.19949995E-01
550	1.21738492E+00	2.21342695E-01

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GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
551	1.22734009E+00	2.22747748E-01
552	1.23739221E+00	2.24165255E-01
553	1.24754212E+00	2.25595319E-01
554	1.25779077E+00	2.27038045E-01
555	1.26813912E+00	2.28493536E-01
556	1.27858816E+00	2.29961899E-01
557	1.28913885E+00	2.31443240E-01
558	1.29979218E+00	2.32937667E-01
559	1.31054917E+00	2.34445289E-01
560	1.32141081E+00	2.35966216E-01
561	1.33237813E+00	2.37500559E-01
562	1.34345217E+00	2.39048428E-01
563	1.35463395E+00	2.40609938E-01
564	1.36592454E+00	2.42185203E-01
565	1.37732500E+00	2.43774337E-01
566	1.38883640E+00	2.45377456E-01
567	1.40045982E+00	2.46994678E-01
568	1.41219637E+00	2.48626121E-01
569	1.42404714E+00	2.50271905E-01
570	1.43601325E+00	2.51932150E-01
571	1.44809584E+00	2.53606977E-01
572	1.46029604E+00	2.55296511E-01
573	1.47261501E+00	2.57000874E-01
574	1.48505390E+00	2.58720192E-01
575	1.49761390E+00	2.60454591E-01
576	1.51029619E+00	2.62204199E-01
577	1.52310197E+00	2.63969145E-01
578	1.53603245E+00	2.65749553E-01
579	1.54908835E+00	2.67545570E-01
580	1.56227241E+00	2.69357312E-01
581	1.57558438E+00	2.71184920E-01
582	1.58902602E+00	2.73028526E-01
583	1.60259861E+00	2.74888269E-01
584	1.61630342E+00	2.76764285E-01
585	1.63014177E+00	2.78656712E-01
586	1.64411495E+00	2.80565692E-01
587	1.65822431E+00	2.82491364E-01
588	1.67247117E+00	2.84433873E-01
589	1.68685620E+00	2.86393362E-01
590	1.70138286E+00	2.88369975E-01
591	1.71605042E+00	2.90363861E-01
592	1.73086079E+00	2.92375167E-01
593	1.74581597E+00	2.94404043E-01
594	1.76091679E+00	2.96450639E-01
595	1.77616489E+00	2.98515107E-01
596	1.79156171E+00	3.00597603E-01
597	1.80710873E+00	3.02698279E-01
598	1.82280742E+00	3.04817295E-01
599	1.83865929E+00	3.06954806E-01
600	1.85466584E+00	3.09110974E-01

TABLE VII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
601	1.87082861E+00	3.11285958E-01
602	1.88714913E+00	3.13479923E-01
603	1.90362897E+00	3.15693030E-01
604	1.92026970E+00	3.17925448E-01
605	1.93707292E+00	3.20177342E-01
606	1.95404022E+00	3.22449881E-01
607	1.97117323E+00	3.24740236E-01
608	1.98847359E+00	3.27051578E-01
609	2.00594297E+00	3.29383082E-01
610	2.02358302E+00	3.31734922E-01
611	2.04139545E+00	3.34107275E-01
612	2.05938195E+00	3.36500319E-01
613	2.07754427E+00	3.38914236E-01
614	2.09588412E+00	3.41349206E-01
615	2.11440329E+00	3.43805413E-01
616	2.13310354E+00	3.46283043E-01
617	2.15198668E+00	3.48782282E-01
618	2.17105451E+00	3.51303319E-01
619	2.19030987E+00	3.53846344E-01
620	2.20975162E+00	3.56411551E-01
621	2.22938461E+00	3.58999133E-01
622	2.24920976E+00	3.61609286E-01
623	2.26922895E+00	3.64242207E-01
624	2.28944125E+00	3.66898097E-01
625	2.30985723E+00	3.69577156E-01
626	2.33047023E+00	3.72279589E-01
627	2.35128511E+00	3.75005600E-01
628	2.37230339E+00	3.77755396E-01
629	2.39352859E+00	3.80529188E-01
630	2.41496126E+00	3.83327185E-01
631	2.43660398E+00	3.86149601E-01
632	2.45845833E+00	3.88996651E-01
633	2.48052793E+00	3.91868552E-01
634	2.50281341E+00	3.94765523E-01
635	2.52531744E+00	3.97687785E-01
636	2.54804218E+00	4.00635562E-01
637	2.57098933E+00	4.03609079E-01
638	2.59416263E+00	4.06608563E-01
639	2.61756282E+00	4.09634244E-01
640	2.64119266E+00	4.12696354E-01
641	2.66505445E+00	4.15765126E-01
642	2.68915051E+00	4.18870796E-01
643	2.71348317E+00	4.22003604E-01
644	2.73805430E+00	4.25163789E-01
645	2.76286778E+00	4.28351594E-01
646	2.78792453E+00	4.31567264E-01
647	2.81322747E+00	4.34811047E-01
648	2.83877909E+00	4.38083192E-01
649	2.86458135E+00	4.41383952E-01
650	2.89063827E+00	4.44713581E-01

TABLE VII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
651	2.91695090E+00	4.48072334E-01
652	2.94352219E+00	4.51460459E-01
653	2.97035465E+00	4.54878200E-01
654	2.99745079E+00	4.58325809E-01
655	3.02481316E+00	4.61803536E-01
656	3.05244434E+00	4.65311637E-01
657	3.08034691E+00	4.68850367E-01
658	3.10852351E+00	4.72419986E-01
659	3.13697678E+00	4.76020756E-01
660	3.16570940E+00	4.79652940E-01
661	3.19472408E+00	4.83316805E-01
662	3.22402355E+00	4.87012620E-01
663	3.25361056E+00	4.90740657E-01
664	3.28348790E+00	4.94501190E-01
665	3.31365839E+00	4.98294495E-01
666	3.34412487E+00	5.02120952E-01
667	3.37489022E+00	5.05980543E-01
668	3.40595733E+00	5.09873852E-01
669	3.43732914E+00	5.13801068E-01
670	3.46900861E+00	5.17762479E-01
671	3.50099872E+00	5.21758379E-01
672	3.53330251E+00	5.25789063E-01
673	3.56592301E+00	5.29854830E-01
674	3.59886351E+00	5.33955980E-01
675	3.63212652E+00	5.38092818E-01
676	3.66571579E+00	5.42265649E-01
677	3.69963429E+00	5.46474785E-01
678	3.73388524E+00	5.50720337E-01
679	3.76847186E+00	5.55003220E-01
680	3.80339745E+00	5.59323154E-01
681	3.83866529E+00	5.63680659E-01
682	3.87427873E+00	5.68076060E-01
683	3.91024115E+00	5.72509685E-01
684	3.94655595E+00	5.76981864E-01
685	3.98322657E+00	5.81492930E-01
686	4.02025649E+00	5.86043220E-01
687	4.05764922E+00	5.90633074E-01
688	4.09540830E+00	5.95262835E-01
689	4.13353733E+00	5.99932849E-01
690	4.17203991E+00	6.04643465E-01
691	4.21091971E+00	6.09395037E-01
692	4.25018041E+00	6.14187920E-01
693	4.28982574E+00	6.19022474E-01
694	4.32985948E+00	6.23899060E-01
695	4.37028542E+00	6.28818046E-01
696	4.41110741E+00	6.33779800E-01
697	4.45232933E+00	6.38784695E-01
698	4.49395510E+00	6.43833109E-01
699	4.53593868E+00	6.48925419E-01
700	4.57843408E+00	6.54062011E-01

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GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
701	4.62129532E+00	6.59243270E-01
702	4.66457650E+00	6.64469588E-01
703	4.70828174E+00	6.69741357E-01
704	4.75241520E+00	6.75058977E-01
705	4.79698109E+00	6.80422849E-01
706	4.84198365E+00	6.85833378E-01
707	4.88742717E+00	6.91290972E-01
708	4.93331600E+00	6.96796045E-01
709	4.97965450E+00	7.02349013E-01
710	5.02644711E+00	7.07950297E-01
711	5.07369828E+00	7.13600321E-01
712	5.12141254E+00	7.19299514E-01
713	5.16959443E+00	7.25048307E-01
714	5.21824856E+00	7.30847137E-01
715	5.26737958E+00	7.36696444E-01
716	5.31699218E+00	7.42596674E-01
717	5.36709112E+00	7.48548273E-01
718	5.41768117E+00	7.54551696E-01
719	5.46876719E+00	7.60607398E-01
720	5.52035406E+00	7.66715841E-01
721	5.57244671E+00	7.72877491E-01
722	5.62505014E+00	7.79092817E-01
723	5.67816938E+00	7.85362293E-01
724	5.73180952E+00	7.91686398E-01
725	5.78597570E+00	7.98065614E-01
726	5.84067312E+00	8.04500429E-01
727	5.89590701E+00	8.10991335E-01
728	5.95168267E+00	8.17538829E-01
729	6.00800546E+00	8.24143410E-01
730	6.06488077E+00	8.30805585E-01
731	6.12231407E+00	8.37525865E-01
732	6.18031037E+00	8.44304764E-01
733	6.23887674E+00	8.51142902E-01
734	6.29801730E+00	8.58040504E-01
735	6.35773824E+00	8.64998199E-01
736	6.41804529E+00	8.72017023E-01
737	6.47894425E+00	8.79096913E-01
738	6.54044097E+00	8.86238615E-01
739	6.60254138E+00	8.93442677E-01
740	6.66525143E+00	9.00709655E-01
741	6.72857720E+00	9.08040108E-01
742	6.79252474E+00	9.15434601E-01
743	6.85710022E+00	9.22893703E-01
744	6.92230935E+00	9.30417991E-01
745	6.98815993E+00	9.38008044E-01
746	7.05465679E+00	9.45664449E-01
747	7.12180685E+00	9.53387797E-01
748	7.18961657E+00	9.61178686E-01
749	7.25809249E+00	9.69037716E-01
750	7.32724123E+00	9.76965497E-01

TABLE VII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

R	R(R)	PSI(R)
751	7.39706945E+00	9.84962643E-01
752	7.46758398E+00	9.93029771E-01
753	7.53879133E+00	1.00116751E+00
754	7.61069369E+00	1.00957648E+00
755	7.68531289E+00	1.01765734E+00
756	7.75664094E+00	1.02601071E+00
757	7.83068093E+00	1.03443724E+00
758	7.90546702E+00	1.04293760E+00
759	7.98097944E+00	1.05151244E+00
760	8.05723448E+00	1.06016243E+00
761	8.13423953E+00	1.06888824E+00
762	8.21200202E+00	1.07769055E+00
763	8.29052949E+00	1.08657005E+00
764	8.36982953E+00	1.09552743E+00
765	8.44990093E+00	1.10456339E+00
766	8.53077813E+00	1.11367861E+00
767	8.61244227E+00	1.12287383E+00
768	8.69491017E+00	1.13214976E+00
769	8.77819980E+00	1.14150713E+00
770	8.86222091E+00	1.15094666E+00
771	8.94721467E+00	1.16046909E+00
772	9.03290029E+00	1.17007517E+00
773	9.11958843E+00	1.17976564E+00
774	9.20704950E+00	1.18954128E+00
775	9.29537199E+00	1.19940284E+00
776	9.38456446E+00	1.20935109E+00
777	9.47463557E+00	1.21938682E+00
778	9.56559409E+00	1.22951081E+00
779	9.65744383E+00	1.23972385E+00
780	9.75020872E+00	1.25002676E+00
781	9.84388273E+00	1.26042033E+00
782	9.93848012E+00	1.27090539E+00
783	1.00340099E+01	1.28148275E+00
784	1.01304315E+01	1.29215325E+00
785	1.02279042E+01	1.30291774E+00
786	1.03262876E+01	1.31377705E+00
787	1.04256412E+01	1.32473904E+00
788	1.05259746E+01	1.33578358E+00
789	1.06272977E+01	1.34693251E+00
790	1.07296203E+01	1.35817978E+00
791	1.08329523E+01	1.36952621E+00
792	1.09373040E+01	1.38097272E+00
793	1.10426853E+01	1.39252021E+00
794	1.11491066E+01	1.40416960E+00
795	1.12565733E+01	1.41592180E+00
796	1.13651109E+01	1.42777775E+00
797	1.14747149E+01	1.43973838E+00
798	1.15854010E+01	1.45180464E+00
799	1.16971801E+01	1.46397748E+00
800	1.18100630E+01	1.47625787E+00

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                        TABLE VII

                          GOLD

        LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE
        R(R) AND PSI(R) WITH R IN 1/100 BOHR UNITS

       R                R(R)                         PSI(R)

      801          1.19240608E+01               1.48864679E+00
      802          1.20391845E+01               1.50114521E+00
      803          1.21554456E+01               1.51375412E+00
      804          1.22728532E+01               1.52647453E+00
      805          1.23914250E+01               1.53930745E+00
      806          1.25111664E+01               1.55225389E+00
      807          1.26320911E+01               1.56531489E+00
      808          1.27542111E+01               1.57849148E+00
      809          1.28775383E+01               1.59178471E+00
      810          1.30020846E+01               1.60519563E+00
      811          1.31278624E+01               1.61872533E+00
      812          1.32548839E+01               1.63237487E+00
      813          1.33831616E+01               1.64614534E+00
      814          1.35127080E+01               1.66003783E+00
      815          1.36435357E+01               1.67405347E+00
      816          1.37756578E+01               1.68819335E+00
      817          1.39090369E+01               1.70245862E+00
      818          1.40433364E+01               1.71685041E+00
      819          1.41799193E+01               1.73136988E+00
      820          1.43173490E+01               1.74601817E+00
      821          1.44561390E+01               1.76079647E+00
      822          1.45963329E+01               1.77570595E+00
      823          1.47379545E+01               1.79074731E+00
      824          1.48802076E+01               1.80592325E+00
      825          1.50251763E+01               1.82123349E+00
      826          1.51709748E+01               1.83667975E+00
      827          1.53182173E+01               1.85226328E+00
      828          1.54669184E+01               1.86798531E+00
      829          1.56170926E+01               1.88384712E+00
      830          1.57687548E+01               1.89984997E+00
TIME,  0 MINUTES AND  59 SECONDS
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TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE FUNCTIONS R(R) AND PSI(R)PSI(R)* WITH R IN 1/100 BOHR UNITS.

R	PSI(R)PSI(R)*
1	5.93189234E-01
2	1.96805980E+00
3	9.31935645E-01
4	2.17757251E-01
5	1.30393549E-03
6	6.66528726E-02
7	1.80637782E-01
8	2.39520379E-01
9	2.29074490E-01
10	1.74401300E-01
11	1.06943654E-01
12	4.96832492E-02
13	1.37235222E-02
14	3.25189885E-04
15	4.76931949E-03
16	1.98951260E-02
17	3.86570303E-02
18	5.55493358E-02
19	6.71471257E-02
20	7.20248897E-02
21	7.03437908E-02
22	6.33455041E-02
23	5.27855353E-02
24	4.05639775E-02
25	2.83876116E-02
26	1.76030287E-02
27	9.11333672E-03
28	3.37957028E-03
29	4.73897770E-04
30	1.62456085E-04
31	1.99928893E-03
32	5.41764579E-03
33	9.51020787E-03
34	1.45931197E-02
35	1.92523769E-02
36	2.33730602E-02
37	2.66534051E-02
38	2.89064634E-02
39	3.00523853E-02
40	3.01042771E-02
41	2.91502886E-02
42	2.73341563E-02
43	2.48359549E-02
44	2.18543338E-02
45	1.85910878E-02
46	1.52335363E-02
47	1.19698880E-02
48	8.93252076E-03
49	6.24397008E-03
50	3.99027210E-03

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE FUNCTIONS R(R) AND PSI(R)PSI(R)* WITH R IN 1/100 BOHR UNITS.

R	PSI(R)PSI(R)*
51	2.22627863E-03
52	9.77523835E-04
53	2.43235664E-04
54	1.13352901E-07
55	2.06535388E-04
56	8.06912938E-04
57	1.73595722E-03
58	2.92263203E-03
59	4.29401250E-03
60	5.77791422E-03
61	7.30599824E-03
62	8.81558567E-03
63	1.02512446E-02
64	1.15658299E-02
65	1.27210707E-02
66	1.36877606E-02
67	1.44456088E-02
68	1.49828150E-02
69	1.52954256E-02
70	1.53865301E-02
71	1.52653490E-02
72	1.49462598E-02
73	1.44478016E-02
74	1.37916924E-02
75	1.30018862E-02
76	1.21036934E-02
77	1.11229776E-02
78	1.00854430E-02
79	9.01601628E-03
80	7.93932759E-03
81	6.87428876E-03
82	5.84376643E-03
83	4.86434435E-03
84	3.95116835E-03
85	3.11636597E-03
86	2.37153236E-03
87	1.72277342E-03
88	1.17579745E-03
89	7.33546478E-04
90	3.96859068E-04
91	1.64656768E-04
92	3.41470704E-05
93	1.03645815E-06
94	5.97478278E-05
95	2.03637333E-04
96	4.25206442E-04
97	7.16305717E-04
98	1.06832749E-03
99	1.47238524E-03
100	1.91947812E-03

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE FUNCTIONS R(R) AND PSI(R)PSI(R)* WITH R IN 1/100 BOHR UNITS.

R	PSI(R)PSI(R)*
101	2.40063947E-03
102	2.90706867E-03
103	3.43024630E-03
104	3.96203243E-03
105	4.49474868E-03
106	5.02124463E-03
107	5.53494933E-03
108	6.02990901E-03
109	6.50081198E-03
110	6.94300192E-03
111	7.35248068E-03
112	7.72590192E-03
113	8.06055658E-03
114	8.35435151E-03
115	8.60578232E-03
116	8.81490143E-03
117	8.97228242E-03
118	9.09298149E-03
119	9.17649699E-03
120	9.21172762E-03
121	9.20573014E-03
122	9.16067710E-03
123	9.07781510E-03
124	8.95942410E-03
125	8.80777809E-03
126	8.62530751E-03
127	8.41456358E-03
128	8.17318430E-03
129	7.91836578E-03
130	7.63932842E-03
131	7.34229556E-03
132	7.03046714E-03
133	6.70649877E-03
134	6.37298275E-03
135	6.03243148E-03
136	5.68726308E-03
137	5.33978925E-03
138	4.99220520E-03
139	4.64658147E-03
140	4.30435767E-03
141	3.96833782E-03
142	3.64018731E-03
143	3.32043128E-03
144	3.01095423E-03
145	2.71300086E-03
146	2.42757794E-03
147	2.15595704E-03
148	1.89857206E-03
149	1.65655352E-03
150	1.43017331E-03

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE FUNCTIONS R(R) AND PSI(R)PSI(R)* WITH R IN 1/100 BOHR UNITS.

R	PSI(R)PSI(R)*
151	1.22001000E-03
152	1.02642450E-03
153	8.49673025E-04
154	6.89908271E-04
155	5.47195770E-04
156	4.21510301E-04
157	3.12747336E-04
158	2.20723466E-04
159	1.45207755E-04
160	8.58779769E-05
161	4.73767103E-05
162	1.42922604E-05
163	1.16937395E-06
164	2.51473579E-06
165	1.78022262E-05
166	4.64779264E-05
167	8.79648629E-05
168	1.41667494E-04
169	2.06975863E-04
170	2.83269639E-04
171	3.69921655E-04
172	4.66301370E-04
173	5.71777970E-04
174	6.85723237E-04
175	8.07514155E-04
176	9.36535286E-04
177	1.07218088E-03
178	1.21335682E-03
179	1.36098227E-03
180	1.51239116E-03
181	1.66935352E-03
182	1.82947652E-03
183	1.99290544E-03
184	2.15912443E-03
185	2.32765713E-03
186	2.49804715E-03
187	2.66935839E-03
188	2.84267529E-03
189	3.01610295E-03
190	3.18976713E-03
191	3.36331419E-03
192	3.53641039E-03
193	3.70874422E-03
194	3.88002107E-03
195	4.04996784E-03
196	4.21833007E-03
197	4.38487199E-03
198	4.54937597E-03
199	4.71154207E-03
200	4.87148741E-03

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE FUNCTIONS R(R) AND PSI(R)PSI(R)* WITH R IN 1/100 BOHR UNITS.

R	PSI(R)PSI(R)*
201	5.02874565E-03
202	5.18326636E-03
203	5.33491440E-03
204	5.48356936E-03
205	5.62912486E-03
206	5.77148798E-03
207	5.91057860E-03
208	6.04632878E-03
209	6.17868215E-03
210	6.30759329E-03
211	6.43302714E-03
212	6.55495838E-03
213	6.67337088E-03
214	6.78825713E-03
215	6.89961765E-03
216	7.00746054E-03
217	7.11130086E-03
218	7.21256020E-03
219	7.31006619E-03
220	7.4040519[illegible]E-03
221	7.49455581E-03
222	7.58102071E-03
223	7.66539398E-03
224	7.74652641E-03
225	7.82417292E-03
226	7.89859114E-03
227	7.96994165E-03
228	8.03828742E-03
229	8.10359372E-03
230	8.16622762E-03
231	8.22505782E-03
232	8.28295440E-03
233	8.33728854E-03
234	8.38903232E-03
235	8.43825849E-03
236	8.48504028E-03
237	8.52945122E-03
238	8.57156497E-03
239	8.61145515E-03
240	8.64919518E-03
241	8.68435817E-03
242	8.71851690E-03
243	8.75024316E-03
244	8.78010869E-03
245	8.80813405E-03
246	8.83453907E-03
247	8.85924261E-03
248	8.88236257E-03
249	8.90376574E-03
250	8.92411782E-03

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE FUNCTIONS R(R) AND PSI(R)PSI(R)* WITH R IN 1/100 BOHR UNITS.

251	8.94288332E-03
252	8.96032552E-03
253	8.97650645E-03
254	8.99148686E-03
255	9.00532617E-03
256	9.01808245E-03
257	9.02931243E-03
258	9.04057144E-03
259	9.05041345E-03
260	9.05939102E-03
261	9.06755532E-03
262	9.07495611E-03
263	9.08164179E-03
264	9.08765933E-03
265	9.09305433E-03
266	9.09787103E-03
267	9.10215230E-03
268	9.10593965E-03
269	9.10927325E-03
270	9.11219197E-03
271	9.11473337E-03
272	9.11693371E-03
273	9.11882801E-03
274	9.12045002E-03
275	9.12133220E-03
276	9.12300611E-03
277	9.12400167E-03
278	9.12484795E-03
279	9.12557279E-03
280	9.12620294E-03
281	9.12676404E-03
282	9.12728067E-03
283	9.12777635E-03
284	9.12827361E-03
285	9.12879394E-03
286	9.12935789E-03
287	9.12998503E-03
288	9.13069402E-03
289	9.13150260E-03
290	9.13242762E-03
291	9.13349507E-03
292	9.13469009E-03
293	9.13605702E-03
294	9.13759938E-03
295	9.13932990E-03
296	9.14126055E-03
297	9.14340259E-03
298	9.14576651E-03
299	9.14836212E-03
300	9.15119855E-03

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE FUNCTIONS R(R) AND PSI(R)PSI(R)* WITH R IN 1/100 BOHR UNITS.

R	PSI(R)PSI(R)*
301	9.15427637E-03
302	9.15760376E-03
303	9.16118877E-03
304	9.16503940E-03
305	9.16916351E-03
306	9.17356894E-03
307	9.17826340E-03
308	9.18325454E-03
309	9.18854994E-03
310	9.19415711E-03
311	9.20009349E-03
312	9.20633647E-03
313	9.21292334E-03
314	9.21985139E-03
315	9.22712779E-03
316	9.23475972E-03
317	9.24275429E-03
318	9.25111854E-03
319	9.25985951E-03
320	9.26898418E-03
321	9.27849948E-03
322	9.28841234E-03
323	9.29872964E-03
324	9.30945824E-03
325	9.32060496E-03
326	9.33217664E-03
327	9.34418005E-03
328	9.35652199E-03
329	9.36950923E-03
330	9.38234852E-03
331	9.39654662E-03
332	9.41091028E-03
333	9.42564625E-03
334	9.44036130E-03
335	9.45656217E-03
336	9.47275563E-03
337	9.48944848E-03
338	9.50664748E-03
339	9.52435947E-03
340	9.54259125E-03
341	9.56134969E-03
342	9.58054166E-03
343	9.60047405E-03
344	9.62085381E-03
345	9.64178789E-03
346	9.66328330E-03
347	9.68534708E-03
348	9.70798630E-03
349	9.73120809E-03
350	9.75501962E-03

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE FUNCTIONS R(R) AND PSI(R)PSI(R)* WITH R IN 1/100 BOHR UNITS.

R	PSI(R)PSI(R)*
351	9.77942811E-03
352	9.80444082E-03
353	9.83006507E-03
354	9.85630829E-03
355	9.88317786E-03
356	9.91068132E-03
357	9.93882621E-03
358	9.96762020E-03
359	9.99707097E-03
360	1.00271863E-02
361	1.00579741E-02
362	1.00894422E-02
363	1.01215987E-02
364	1.01544516E-02
365	1.01880092E-02
366	1.02222798E-02
367	1.02572716E-02
368	1.02929932E-02
369	1.03294531E-02
370	1.03666600E-02
371	1.04046226E-02
372	1.04433498E-02
373	1.04828506E-02
374	1.05231340E-02
375	1.05642093E-02
376	1.06060858E-02
377	1.06487729E-02
378	1.06922801E-02
379	1.07366173E-02
380	1.07817941E-02
381	1.08278205E-02
382	1.08747066E-02
383	1.09224627E-02
384	1.09710990E-02
385	1.10206262E-02
386	1.10710547E-02
387	1.11223955E-02
388	1.11746594E-02
389	1.12278577E-02
390	1.12820015E-02
391	1.13371023E-02
392	1.13931716E-02
393	1.14502213E-02
394	1.15082633E-02
395	1.15673096E-02
396	1.16273726E-02
397	1.16884648E-02
398	1.17505988E-02
399	1.18137874E-02
400	1.18780437E-02

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE FUNCTIONS R(R) AND PSI(R)PSI(R)* WITH R IN 1/100 BOHR UNITS.

R	PSI(R)PSI(R)*
401	1.19433810E-02
402	1.20093126E-02
403	1.20773522E-02
404	1.21460137E-02
405	1.22158110E-02
406	1.22867586E-02
407	1.23598702E-02
408	1.24321625E-02
409	1.25066484E-02
410	1.25823439E-02
411	1.26592643E-02
412	1.27374252E-02
413	1.28168426E-02
414	1.28975326E-02
415	1.29795116E-02
416	1.30627962E-02
417	1.31474033E-02
418	1.32335501E-02
419	1.33206540E-02
420	1.34093328E-02
421	1.34994045E-02
422	1.35908872E-02
423	1.36837997E-02
424	1.37781606E-02
425	1.38739893E-02
426	1.39713051E-02
427	1.40701279E-02
428	1.41704776E-02
429	1.42723747E-02
430	1.43758400E-02
431	1.44808944E-02
432	1.45875594E-02
433	1.46958567E-02
434	1.48058083E-02
435	1.49174367E-02
436	1.50307647E-02
437	1.51458154E-02
438	1.52626123E-02
439	1.53811794E-02
440	1.55015409E-02
441	1.56237213E-02
442	1.57477460E-02
443	1.58736402E-02
444	1.60014293E-02
445	1.61311413E-02
446	1.62628011E-02
447	1.63954365E-02
448	1.65320751E-02
449	1.66697448E-02
450	1.68094741E-02

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE FUNCTIONS R(R) AND PSI(R)PSI(R)* WITH R IN 1/100 BOHR UNITS.

R	PSI(R)PSI(R)*
451	1.69512920E-02
452	1.70952278E-02
453	1.72413114E-02
454	1.73895732E-02
455	1.75400439E-02
456	1.76927543E-02
457	1.78477379E-02
458	1.80050255E-02
459	1.81646504E-02
460	1.83266460E-02
461	1.84910463E-02
462	1.86578857E-02
463	1.88271994E-02
464	1.89990228E-02
465	1.91733922E-02
466	1.93503444E-02
467	1.95299168E-02
468	1.97121472E-02
469	1.98970743E-02
470	2.00847374E-02
471	2.02751761E-02
472	2.04684312E-02
473	2.06645436E-02
474	2.08635552E-02
475	2.10655086E-02
476	2.12704463E-02
477	2.14784139E-02
478	2.16894543E-02
479	2.19036135E-02
480	2.21209375E-02
481	2.23414731E-02
482	2.25652679E-02
483	2. 7923702E-02
484	2.30228292E-02
485	2.32556948E-02
486	2.34940178E-02
487	2.37348498E-02
488	2.39792431E-02
489	2.42272511E-02
490	2.44739280E-02
491	2.47343287E-02
492	2.49935091E-02
493	2.52565262E-02
494	2.55234378E-02
495	2.57943025E-02
496	2.60691800E-02
497	2.63481309E-02
498	2.66312171E-02
499	2.69135010E-02
500	2.72100465E-02

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE FUNCTIONS R(R) AND PSI(R)PSI(R)* WITH R IN 1/100 BOHR UNITS.

R	PSI(R)PSI(R)*
501	2.75059182E-02
502	2.78051819E-02
503	2.81109046E-02
504	2.84201541E-02
505	2.87339997E-02
506	2.90525115E-02
507	2.93757609E-02
508	2.97058204E-02
509	3.00367640E-02
510	3.03746664E-02
511	3.07176039E-02
512	3.10656539E-02
513	3.14138952E-02
514	3.17774079E-02
515	3.21412733E-02
516	3.25105740E-02
517	3.28853941E-02
518	3.32658192E-02
519	3.36519360E-02
520	3.40438328E-02
521	3.44415994E-02
522	3.48453271E-02
523	3.52551086E-02
524	3.56710382E-02
525	3.60932118E-02
526	3.65217267E-02
527	3.69566821E-02
528	3.73931786E-02
529	3.78463136E-02
530	3.83012063E-02
531	3.87629474E-02
532	3.92316494E-02
533	3.97074217E-02
534	4.01903756E-02
535	4.06806239E-02
536	4.11782817E-02
537	4.16834656E-02
538	4.21962946E-02
539	4.27168893E-02
540	4.32453724E-02
541	4.37918689E-02
542	4.43265055E-02
543	4.48794114E-02
544	4.54407175E-02
545	4.60105575E-02
546	4.65890667E-02
547	4.71763831E-02
548	4.77726469E-02
549	4.83780004E-02
550	4.89925888E-02

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE FUNCTIONS R(R) AND PSI(R)PSI(R)* WITH R IN 1/100 BOHR UNITS.

R	PSI(R)PSI(R)*
551	4.96165592E-02
552	5.02500615E-02
553	5.08932481E-02
554	5.15462738E-02
555	5.22092960E-02
556	5.28824749E-02
557	5.35659733E-02
558	5.42599568E-02
559	5.49645937E-02
560	5.56800552E-02
561	5.64065155E-02
562	5.71441511E-02
563	5.78931425E-02
564	5.86536724E-02
565	5.94259271E-02
566	6.02100959E-02
567	6.10063709E-02
568	6.18149481E-02
569	6.26360264E-02
570	6.34698081E-02
571	6.43164990E-02
572	6.51763085E-02
573	6.60494493E-02
574	6.69361378E-02
575	6.78365942E-02
576	6.87510422E-02
577	6.96797095E-02
578	7.06228276E-02
579	7.15806319E-02
580	7.25533617E-02
581	7.35412606E-02
582	7.45445763E-02
583	7.55635605E-02
584	7.65984693E-02
585	7.76495633E-02
586	7.87171074E-02
587	7.98013710E-02
588	8.09026282E-02
589	8.20211576E-02
590	8.31572427E-02
591	8.43111719E-02
592	8.54832384E-02
593	8.66737403E-02
594	8.78829911E-02
595	8.91112693E-02
596	9.03589185E-02
597	9.16262484E-02
598	9.29135831E-02
599	9.42212530E-02
600	9.55495941E-02

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERG'S. RADIAL WAVE FUNCTIONS R(R) AND PSI(R)PSI(R)* WITH R IN 1/100 BOHR UNITS.

R	PSI(R)PSI(R)*
601	9.68989478E-02
602	9.82696618E-02
603	9.96620895E-02
604	1.01076590E-01
605	1.02513530E-01
606	1.03973281E-01
607	1.05456221E-01
608	1.06962735E-01
609	1.08493214E-01
610	1.10048058E-01
611	1.11627671E-01
612	1.13232465E-01
613	1.14862859E-01
614	1.16519280E-01
615	1.18202162E-01
616	1.19911946E-01
617	1.21649080E-01
618	1.23414022E-01
619	1.25207235E-01
620	1.27029194E-01
621	1.28880377E-01
622	1.30761275E-01
623	1.32672385E-01
624	1.34614213E-01
625	1.36587274E-01
626	1.38592092E-01
627	1.40629200E-01
628	1.42699139E-01
629	1.44802463E-01
630	1.46939731E-01
631	1.49111514E-01
632	1.51318394E-01
633	1.53560962E-01
634	1.55839816E-01
635	1.58155574E-01
636	1.60508854E-01
637	1.62900289E-01
638	1.65330524E-01
639	1.67800214E-01
640	1.70310026E-01
641	1.72860640E-01
642	1.75452744E-01
643	1.78087042E-01
644	1.80764247E-01
645	1.83485088E-01
646	1.86250303E-01
647	1.89060647E-01
648	1.91916884E-01
649	1.94819793E-01
650	1.97770169E-01

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE FUNCTIONS R(R) AND PSI(R)PSI(R)* WITH R IN 1/100 BOHR UNITS.

R	PSI(R)PSI(R)*
651	2.00768817E-01
652	2.03816546E-01
653	2.06914177E-01
654	2.10062547E-01
655	2.13262506E-01
656	2.16514919E-01
657	2.19820667E-01
658	2.23130643E-01
659	2.26595760E-01
660	2.30056943E-01
661	2.33595134E-01
662	2.37131292E-01
663	2.40826392E-01
664	2.44531426E-01
665	2.48297403E-01
666	2.52125350E-01
667	2.56016310E-01
668	2.59971345E-01
669	2.63991537E-01
670	2.68077985E-01
671	2.72231806E-01
672	2.76454139E-01
673	2.80746141E-01
674	2.85103987E-01
675	2.89543880E-01
676	2.94052034E-01
677	2.98634690E-01
678	3.03293109E-01
679	3.08028574E-01
680	3.12842390E-01
681	3.17735886E-01
682	3.22710410E-01
683	3.27767340E-01
684	3.32908071E-01
685	3.38134027E-01
686	3.43446655E-01
687	3.48847428E-01
688	3.54337842E-01
689	3.59919423E-01
690	3.65593720E-01
691	3.71362311E-01
692	3.77226801E-01
693	3.83188823E-01
694	3.89250037E-01
695	3.95412135E-01
696	4.01676835E-01
697	4.08045887E-01
698	4.14521072E-01
699	4.21104200E-01
700	4.27797114E-01

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE FUNCTIONS R(R) AND PSI(R)PSI(R)* WITH R IN 1/100 BOHR UNITS.

R	PSI(R)PSI(R)*
701	4.34601689E-01
702	4.41519833E-01
703	4.48553486E-01
704	4.55704623E-01
705	4.62975254E-01
706	4.70367422E-01
707	4.77883208E-01
708	4.85524728E-01
709	4.93204136E-01
710	5.01193623E-01
711	5.09225419E-01
712	5.17391790E-01
713	5.25695047E-01
714	5.34137537E-01
715	5.42721651E-01
716	5.51449820E-01
717	5.60324517E-01
718	5.69348261E-01
719	5.78523614E-01
720	5.87853181E-01
721	5.97339616E-01
722	6.06985617E-01
723	6.16793931E-01
724	6.26767353E-01
725	6.36908724E-01
726	6.47220941E-01
727	6.57706946E-01
728	6.68369736E-01
729	6.79212360E-01
730	6.90237921E-01
731	7.01449575E-01
732	7.12850535E-01
733	7.24444070E-01
734	7.36233507E-01
735	7.48222231E-01
736	7.60413688E-01
737	7.72811392E-01
738	7.85418882E-01
739	7.98239817E-01
740	8.11277885E-01
741	8.24536833E-01
742	8.38020508E-01
743	8.51732788E-01
744	8.65677638E-01
745	8.79859091E-01
746	8.94231251E-01
747	9.08948292E-01
748	9.23864466E-01
749	9.39034095E-01
750	9.54461583E-01

TABLE VIII

GOLD

LOWEST ENERGY STATE IS 1.194 RYDBERGS. RADIAL WAVE FUNCTIONS R(R) AND PSI(R)PSI(R)* WITH R IN 1/100 BOHR UNITS.

R	PSI(R)PSI(R)*
751	9.70151407E-01
752	9.86108126E-01
753	1.00233638E+00
754	1.01834089E+00
755	1.03562645E+00
756	1.05269797E+00
757	1.07006041E+00
758	1.08771884E+00
759	1.10567842E+00
760	1.12394438E+00
761	1.14252208E+00
762	1.16141693E+00
763	1.18063443E+00
764	1.20018034E+00
765	1.22006025E+00
766	1.24028004E+00
767	1.26034564E+00
768	1.28176309E+00
769	1.30303852E+00
770	1.32457820E+00
771	1.34668850E+00
772	1.36907590E+00
773	1.39184698E+00
774	1.41500846E+00
775	1.43856717E+00
776	1.46253006E+00
777	1.48690421E+00
778	1.51169683E+00
779	1.53691524E+00
780	1.56256690E+00
781	1.58865941E+00
782	1.61520050E+00
783	1.64219804E+00
784	1.66956003E+00
785	1.69759463E+00
786	1.72601013E+00
787	1.75491498E+00
788	1.78431777E+00
789	1.81422724E+00
790	1.84465232E+00
791	1.87560204E+00
792	1.90708566E+00
793	1.93911255E+00
794	1.97169227E+00
795	2.00483455E+00
796	2.03854930E+00
797	2.07284660E+00
798	2.10773671E+00
799	2.14323007E+00
800	2.17933731E+00

TABLE VIII

GOLD

LOWEST ENERGY STATE IS -1.194 RYDBERGS. RADIAL WAVE FUNCTIONS R(R) AND PSI(R)PSI(R)* WITH R IN 1/100 BOHR UNITS.

R	PSI(R)PSI(R)*
801	2.21606926E+00
802	2.25343693E+00
803	2.29145154E+00
804	2.33012449E+00
805	2.36946742E+00
806	2.40949214E+00
807	2.45021070E+00
808	2.49163534E+00
809	2.53377855E+00
810	2.57665303E+00
811	2.62027169E+00
812	2.66464771E+00
813	2.70979446E+00
814	2.75570560E+00
815	2.80245500E+00
816	2.84999680E+00
817	2.89836536E+00
818	2.94757534E+00
819	2.99764165E+00
820	3.04857946E+00
821	3.10040421E+00
822	3.15313165E+00
823	3.20677773E+00
824	3.26135880E+00
825	3.31689143E+00
826	3.37339252E+00
827	3.43037925E+00
828	3.48936913E+00
829	3.54937997E+00
830	3.60942991E+00

APPENDIX IV

FORTRAN COMPUTATIONAL PROGRAMS

THE FOLLOWING PROGRAMS WERE USED IN THE COMPILATION OF DATA AND RESULTS ACHIEVED. THESE PROGRAMS ARE PREPARED IN FORTRAN 60 LANGUAGE FOR THE 1604 CONTROL DATA COMPUTOR. THE READER SHOULD KEEP IN MIND THESE PROGRAMS ARE THE END PRODUCTS OF MANY SMALLER PROGRAMS AND BUILT FOR FLEXIBILITY. AS A RESULT SOME OF THE FORTRAN PROGRAMMING MAY NOT BE THE MOST EFFICIENT. THE GRAPH ROUTINE UTILIZED THE CONTROL DATA 160 COMPUTOR, CONTROL DATA 165 PLOTTER AND CALIFORNIA COMPUTER PRODUCTS 565 FOR REPRODUCTION.

THE SOLUTION TO THE TRINOMIAL EQUATION FOR SODIUM, CODE NAME BIG ONE, IS INDICATED AT PAGES TO . INCLUDED ARE THE DATA POINTS FOR THE PROKOFIEV POTENTIAL.

THE SOLUTION TO THE CELLULAR CALCULATION FOR GOLD, CODE NAME BOHR-S, USING THE NEW POTENTIAL IS INDICATED AT PAGES TO .

THE SEARCH FOR THE VALUES OF THE PARAMETERS MEETING THE IONIZATION ENERGY, CODE NAME SEARCH, IS INDICATED AT PAGES TO . IT IS NOTED THAT THE CELLULAR CALCULATION IS MADE ONCE THE BOUNDARY CONDITIONS ARE SATISFIED.

THE GRAPH ROUTINE FOR THE PLOTTING OF R(R) FROM KNOWN POTENTIALS IS INDICATED AT PAGES TO .

THE GRAPH ROUTINE FOR THE PLOTTING OF R(R), PSI(R) AND PSI(R)PSI(R)* FOR THE NEW POTENTIAL IS INDICATED AT PAGES TO .

```
..JOB*MUSORRAFITI AND SLAZAK     THESIS    BIG ONE   FEB 1964
      PROGRAM THESIS
     0DIMENSION A(670),Y1(667),Y2(667),Y3(667),Y4(667),
     1Y6(670),Y7(670),Y8(670),F1(1),F2(1),F3(1),F4(1),F5(1),
     2F6(1),F7(1),F8(1),F9(1),F10(1),F11(1),F12(1),F13(1),
     3F14(1),F15(1),BB(20),QQ(20),RR(20),F(2,99),AA(2,99),
     4PEE(1),AB(2,99),STAY(1),PLAY(1),SEE(1),POT(670),
     5V(2,99),W(2,99),X(2,99),VV(2,99),WW(2,99),XX(2,99),
     6G(2,99),BUM(1),DRAY(1),CUM(1),BRAY(1),TEE(1),TUM(1),
     7ABLE(1),DOPE(1),BOZO(1),AC(2,99),BC(2,99),CE(2,20),
     8S(2,99),BOT(670),CAL(18),ITITLE(10),XYZ(667),LABEL(
     910)
      DO 1234 J=1,10
 1234 ITITLE(J)=(8H        )
      DO 191 L=1,667
  191 XYZ(L)=L
      ITITLE(1)=(8H SLAZAK    )
      ITITLE(2)=(8HMUSORRAF)
      ITITLE(3)=(8HITI       )
      ITITLE(4)=(8HSODIUM    )
      ITITLE(5)=(8HEASY=.5   )
      ITITLE(6)=(8HRYDBERGS   )
      READ 111,(A(I),I=1,227)
      READ111,(A(I),I=228,306)
      READ 111,(A(I),I=307,335)
      READ 111,(A(I),I=336,400)
      READ 111,(A(I),I=401,670)
  111 FORMAT(6F10.0)
      EASY=0.25
      PRINT 82,EASY
   82 FORMAT(E20.2)
  884 FORMAT(I10,//////)
  885 FORMAT (1P3E20.8,///)
  886 FORMAT (1PE20.8, /// )
  887 FORMAT (1P5E20.8,///)
  888 FORMAT(1P6E20.8,///)
  889 FORMAT (1P2E20.8    )
      Z=11.0
      H=0.01
   10 DO 20 I=2,666
      ON=I
      I6=I-1
      I2=I+2
      I1=I+1
      F1(1)=-Z
      F2(1)=-(2.*Z*F1(1)-2.*EASY)/6.
      F3(1)=-(2.*Z*F2(1)-2.*EASY*F1(1))/12.
```

```
      F4(1)=-(2.*Z*F3(1)-2.*EASY*F2(1))/20.
      F5(1)=-(2.*Z*F4(1)-2.*EASY*F3(1))/30.
      F6(1)=-(2.*Z*F5(1)-2.*EASY*F4(1))/42.
      F7(1)=-(2.*Z*F6(1)-2.*EASY*F5(1))/56.
      F8(1)=-(2.*Z*F7(1)-2.*EASY*F6(1))/72.
      F9(1)=-(2.*Z*F8(1)-2.*EASY*F7(1))/90.
      F10(1)=-(2.*Z*F9(1)-2.*EASY*F8(1))/110.
      F11(1)=-(2.*Z*F10(1)-2.*EASY*F9(1))/132.
      F12(1)=-(2.*Z*F11(1)-2.*EASY*F10(1))/156.
      F13(1)=-(2.*Z*F12(1)-2.*EASY*F11(1))/182.
      F14(1)=-(2.*Z*F13(1)-2.*EASY*F12(1))/210.
      F15(1)=-(2.*Z*F14(1)-2.*EASY*F13(1))/240.
     0Y1(1)=H+F1(1)*H**2+F2(1)*H**3+F3(1)*H**4+F4(1)*H**5
     1+F5(1)*H**6+F6(1)*H**7+F7(1)*H**8+F8(1)*H**9+F9(1)*H
     2**10+F10(1)*H**11+F11(1)*H**12+F12(1)*H**13+F13(1)*H*
     3*14+F14(1)*H**15+F15(1)*H**16
     0Y2(1)=1.+2.*F1(1)+H+3.*F2(1)*H**2+4.*F3(1)*H**3+5.*F4
     1(1)*H**4+6.*F5(1)*H**5+7.*F6(1)*H**6+8.*F7(1)*H**7+9.
     2*F8(1)*H**8+10.*F9(1)*H**9+11.*F10(1)*H**10+12.*F11(1
     3)*H**11+13.*F12(1)*H**12+14.*F13(1)*H**13+15.*F14(1)*
     4H**14*H**14+16.*F15(1)*H**15
C     THE COEFFICIENTS OF THE LOGARITHMIC FUNCTION
      X4=I
      X1=X4*H-H
      X2=X4*H
      X3=X4*H+H
      T1=(X2*(X3**2)-X3*(X2**2))
      T2=(X1*(X3**2)-X3*(X1**2))
      T3=(X1*(X2**2)-X2*(X1**2))
      T4=(X3**2)-(X2**2)
      T5=(X3**2)-(X1**2)
      T6=(X2**2)-(X1**2)
      T7=X3-X2
      T8=X3-X1
      T9=X2-X1
      P1=T1-T2+T3
      A1=(A(I6)*T1-A(I)*T2+A(I1)*T3)/P1
      A2=-(A(I6)*T4-A(I)*T5+A(I1)*T6)/P1
      A3=(A(I6)*T7-A(I)*T8+A(I1)*T9)/P1
      BB(I)=2.*A1*Z
      QQ(I)=2.*A2*Z-2.*EASY
      RR(I)=2.*Z*A3
      DO 200 J=4,75
      J6=J-1
      J2=J-2
      J3=J-3
      CO=J
```

```
      F(I,1)=-BB(I)/2.
      F(I,2)=-(BB(I)*F(I,1)+QQ(I))/6.
      F(I,3)=-(BB(I)*F(I,2)+QQ(I)*F(I,1)+RR(I))/12.
     0F(I,J)=-(BB(I)*F(I,J6)+QQ(I)*F(I,J2)+RR(I)*F(I,J3))/
     1((CO+1.)*CO)
  200 CONTINUE
      DO 201 J=1,75
      CO=J
      AA(I,J)=(ON*H-H)**CO
  201 CONTINUE
       BAD1=0.0
      DO 202 J=2,75
      J6=J-1
      BAD1=AA(I,J)*F(I,J6)+BAD1
  202 CONTINUE
      BEE(I)=CN*H-H+BAD1
      DO 203 J=1,75
      CO=J
      AB(I,J)=(ON*H)**CO
  203 CONTINUE
      ADD1=0.0
      DO 204 J=2,75
      J6=J-1
      ADD1=AB(I,J)*F(I,J6)+ADD1
  204 CONTINUE
      STAY(I)=ADD1+ON*H
      ADD2=0.0
      DO 205 J=2,75
      CO=J
      ADD2=(CO+1.)*F(I,J)*AB(I,J) +ADD2
  205 CONTINUE
      PLAY(I)=1.+2.*F(I,1)*ON*H+ADD2
      ADD3=0.0
      DO 206 J=2,75
      CO=J
      ADD3=(CO+1.)*(F(I,J)*AA(I,J))+ADD3
  206 CONTINUE
      SEE(I)=1.+2.*F(I,1)*(ON*H-H)+ADD3
      POT(I)=LOGF(ON-1.)-LOGF(1./H)
      BOT(I)=LOGF(CN)-LOGF(1./H)
      V(I,1)=-BB(I)
      VV(I,1)=BB(I)
      AC(I,1)=-BB(I)
      BC(I,1)=BB(I)
      G(I,1)=-BB(I)*POT(I)+BB(I)
      S(I,1)=-BB(I)*BOT(I)+BB(I)
      V(I,2)=-BB(I)*AC(I,1)/2.
```

```
      W(I,1)=0.0
      WW(I,2)=-QQ(I)/2.
      VV(I,2)=-BB(I)*(BC(I,1)/2.-AC(I,1)*3./4.)
      AC(I,2)=V(I,2)
      BC(I,2)=VV(I,2)+WW(I,2)
      G(I,2)=AC(I,2)*POT(I)+BC(I,2)
      S(I,2)=AC(I,2)*BOT(I)+BC(I,2)
      V(I,3)=-BB(I)*AC(I,2)/6.
      W(I,3)=-QQ(I)*AC(I,1)/6.
      VV(I,3)=-BB(I)*(-AC(I,2)*5./36.+BC(I,2)/6.)
      WW(I,3)=-QQ(I)*(-AC(I,1)*5./36.+BC(I,1)/6.)
      XX(I,3)=-RR(I)/6.
      AC(I,3)=V(I,3)+W(I,3)
      BC(I,3)=VV(I,3)+WW(I,3)+XX(I,3)
      G(I,3)=AC(I,3)*POT(I)+BC(I,3)
      S(I,3)=AC(I,3)*BOT(I)+BC(I,3)
      CAL(1)=(BB(I)+AC(I,1))/ON*H
      CAL(2)=BB(I)*S(I,1)+QQ(I)+2.*S(I,2)+3.*AC(I,2)
     0CAL(3)=BB(I)*S(I,2)+QQ(I)*S(I,1)+RR(I)+6.*S(I,3)+5.*
     1AC(I,3)
      DO 256 J=4,75
      CO=J
      J2=J-2
      J3=J-3
     0VV(I,J)=-BB(I)*(-AC(I,J6)*(2.*CO-1.)/(CO*(CO-1.))**2
     1+BC(I,J6)/(CO*(CO-1.)))
     0WW(I,J)=-QQ(I)*(-AC(I,J2)*(2.*CO-1.)/(CO*(CO-1.))**2
     1+BC(I,J2)/(CO*(CO-1.)))
     0XX(I,J)=-RR(I)*(-AC(I,J3)*(2.*CO-1.)/(CO*(CO-1.))**2
     1+BC(I,J3)/(CO*(CO-1.)))
      AC(I,J)=V(I,J)+W(I,J)+X(I,J)
      BC(I,J)=VV(I,J)+WW(I,J)+XX(I,J)
      G(I,J)=AC(I,J)*POT(I)+BC(I,J)
      S(I,J)=BC(I,J)+BOT(I)*AC(I,J)
     0CAL(J)=BB(I)*S(I,J6)+QQ(I)*S(I,J2),+RR(I)*S(I,J3)+
     1CO*(CO-1.)*S(I,J)+(2.*CO-1.)*AC(I,J)
  256 CONTINUE
      ADD4=0.0
      DO 207 J=1,75
      ADD4=G(I,J)*AA(I,J)+ADD4
  207 CONTINUE
      BUM(I)=1.+ADD4
      ADD6=0.0
      DO 209 J=2,75
      J6=J-1
      CO=J
      ADD6=AA(I,J6)*(CO*G(I,J)+AC(I,J))+ADD6
```

```
209 CONTINUE
    CUM(I)=G(I,1)+AC(I,1)+ADD6
    ADD5=0.0
    DO 208 J=1,75
    ADD5=S(I,J)*AB(I,J)+ADD5
208 CONTINUE
    DRAY(I)=1.+ADD5
    ADD7=0.0
    DO 210 J=2,75
    J6=J-1
    CO =J
    ADD7=AB(I,J6)*(CO*S(I,J)+AC(I,J))+ADD7
210 CONTINUE
    BRAY(I)=S(I,1)+AC(I,1)+ADD7
    ADD8=0.0
    DO 211 J=2,75
    CO=J
    J6=J-1
    ADD8=CO*(CO+1.)*F(I,J)*AB(I,J6)+ADD8
211 CONTINUE
    TEE(I)=2.*F(I,1)+ADD8
    ADD9=0.0
    DO 212 J=3,75
    J2=J-2
    CO=J
   0ADD9=AB(I,J2)*(CO*(CO-1.)*S(I,J)+(2.*CO-1.)*AC(I,J))+
   1ADD9
212 CONTINUE
    TUM(I)=AC(I,1)/(ON*H)+2.*S(I,2)+3.*AC(I,2)+ADD9
    DOPE(I)=(BUM(I)*SEE(I)-CUM(I)*BEE(I))
    ABLE(I)=(Y1(I6)*SEE(I)-Y2(I6)*BEE(I))/DOPE(I)
    BOZC(I)=(  Y2(I6)*BUM(I)-Y1(I6)*CUM(I))/DOPE(I)
    AK1=ON*H
    Y1(I )=ABLE(I)*DRAY(I)+BOZC(I)*STAY(I)
    Y2(I )=APLE(I)*BRAY(I)+BOZO(I)*PLAY(I)
    Y3(I )=Y1(I )/AK1
    Y4(I)=Y3(I)-Y2(I)
    Y6(I)=ABLE(I)*TUM(I)+BOZO(I)*TEE(I)
    Y7(I)=-2.*(Z*A(I)/(ON*H)-EASY)*Y1(I)
    PRINT 884,I
    PRINT 888,Y1(I),Y2(I),Y3(I),Y4(I),Y6(I),Y7(I)
    HION=.372
    CE(I)=(-2.*EASY+2.2/(AK1**2)+HION)*310.5
 20 CONTINUE
    LABEL=(4HNO=1)
    CALL GRAPH2(667,XYZ,Y1,8,1,LABEL,ITITLE,0,0,0,0,0,0,0)
    LABEL=(4HNO=2)
```

```
      CALL GRAPH2(667,XYZ,Y2,8,2,LABEL,ITITLE,0,0,0,0,0,0,0)
      LABEL=(4HNO=3)
      CALL GRAPH2(667,XYZ,Y3,8,3,LABEL,ITITLE,0,0,0,0,0,0,0)
      EASY=EASY+0.1
      IF(EASY-.35)10,555,555
  555 END
      END
```

```
1.0000      .98800      .96791      .94582      .92293      .89964
.87612      .85245      .828697     .804873     .78100      .757091
.733154     .709195     .6852181    .66386      .643649     .625396
.608792     .593591     .579591     .566629     .554571     .5433015
.532727     .52277      .513355     .504429     .495942     .487848
.480110     .472694     .465571     .458715     .452104     .445716
.439534     .433542     .427724     .422068     .416562     .411196
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.376812     .372273     .3678103    .36342      .359098     .354841
.350645     .34651      .342422     .338389     .334406     .3304697
.326578     .322728     .318918     .315147     .311413     .307713
.304047     .3004123    .296808     .293234     .289687     .286167
.282673     .279203     .275758     .272334     .268933     .2655529
.262193     .258852     .255530     .2522267    .2489402    .245671
.242417     .2391793    .235956     .232748     .229554     .2263737
.2232064    .220052     .2169095    .213779     .2106602    .2075527
.2044559    .2013696    .1982935    .1952273    .192255     .189323
.186475     .1837074    .181019     .1784073    .175869     .173405
.1710104    .168684     .166425     .1642301    .1620986    .1600285
.1580182    .156066     .154171     .152331     .1505454    .148812
.147130     .145498     .1439152    .1423798    .1408989    .1394474
.1380482    .1366923    .1353786    .1341063    .132874     .1316818
.1305278    .1294115    .128332     .127289     .1262803    .125306
.1243667    .1234597    .122585     .121742     .120930     .1201483
.119396     .1186732    .117979     .1173122    .116673     .116061
.1154745    .114914     .1143789    .1138685    .113382     .112906
.1124110    .1119850    .1115760    .1111759    .1108192    .1104681
.1101228    .1097829    .1094485    .1091194    .10879567   .1084770
.1081634    .1078547    .107551     .107252     .1069578    .1066682
.10638312   .1061025    .1058263    .1055545    .1052869    .105023
.104764     .1045088    .1042575    .1040102    .1037666    .103527
.1032909    .1030585    .1028297    .102605     .1023829    .1021646
.1019498    .1017383    .1015383    .1013250    .1011232    .1009245
.100729     .1005363    .100347     .1001602    .099977     .0997957
.09961769   .0994425    .099270     .0991002    .0989331    .0987687
.0986068    .0984474    .0982906    .0981363    .0979844    .0978349
.0976878    .097543     .097400     .0972604    .09712259   .0969869
.096853     .0967221    .0965929    .0964658    .09634084
.09621788   .0960969    .0959780    .0958611    .095746     .0956329
```

```
.0955217   .0954124   .0953049   .09519928  .0950954   .09499335
.0948930   .0947944   .0946976   .0946024   .09450889  .0944170
.0943268   .09423819  .09415116  .0940657   .0939818   .0938995
.0938186   .0937393   .0936614   .0935849   .09351003  .09343651
.0933643   .0932936   .0932243   .0931564   .0930897   .0930244
.0929604   .0928978   .09283642  .0927763   .0927175   .0926599
.0926035   .0925483   .0924944   .09244165  .09239008  .09233967
.0922904   .09224229  .0921953   .09214944  .0921047   .092061
.0920184   .0919768   .0919364   .091897    .0918586   .09182126
.0917849   .0917496   .09171524  .0916187   .09164948  .09161805
.0915876   .0915581   .0915295   .0915019   .09147504  .0914492
.0914242   .0914002   .0913769   .0913547   .09133323  .09131264
.0912929
.09127397  .09125589  .0912386   .0912217   .0912065   .0911917
.091177    .09116434  .0911518   .09114009  .09112912  .0911189
.091109    .09110068  .0910927   .0910854   .0910788   .0910729
.0910678   .09106338  .09105963  .09105656  .0910542   .09105245
.09106018  .09105879  .09105742  .0910561   .09105462
.09105337  .09105205  .0910507   .09104943  .09104812  .09104684
.0910456   .0910443   .0910430   .0910418   .09104056  .09103934
.09103811  .0910369   .0910357   .0910345   .0910335   .09103218
.09103102  .0910299   .09102872  .09102759  .0910265   .09102535
.0910242   .0910231   .09102205  .09102097  .0910199   .09101884
.09101778  .0910167   .0910157   .0910147   .09101364  .09101262
.0910116   .0910106   .0910096   .0910086   .09100766  .09100669
.09100573  .09100477  .09100383  .09100289  .0910019   .09100103
.0910001   .0909992   .0909983   .0909974   .0909965   .0909956
.09099476  .09099389  .0909930   .09099217  .09099132  .09099048
.09098965  .0909888   .09098798  .09098717  .09098636
.09098556  .09098476  .09098397  .09098319  .09098241  .09098163
.09098087  .09098011  .09097935  .09097860  .09097786  .09097712
.09097639  .09097567  .09097495  .09097423  .09097352  .09097282
.09097212  .09097143  .09097074  .09097006  .09096938  .09096871
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.09096046  .09095686  .09095927  .09095868  .09095809  .09095751
.09095694  .09095636  .09095580  .09095523  .09095468  .09095412
.09095357  .09095303  .09095249  .09095195  .09095142  .09095090
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.09093657  .09093617  .09093577  .09093538  .09093499  .09093460
.09093422  .09093384  .09093346  .09093308  .09093271  .09093235
.09093198  .09093162  .09093126  .09093091  .09093056  .09093021
.09092987  .09092952  .09092919  .09092885  .09092852  .09092819
```

```
.09092786 .09092754 .09092722 .09092690 .09092659 .09092628
.09092597 .09092567 .09092536 .09092506 .09092477 .09092448
.09092419 .09092390 .09092361 .09092333 .09092305 .09092278
.09092250 .09092223 .09092196 .09092170 .09092144 .09092118
.09092092 .09092066 .09092041 .09092016 .09091992 .09091967
.09091943 .09091919 .09091896 .09091872 .09091849 .09091826
.09091804 .09091781 .09091759 .09091737 .09091716 .09091694
.09091673 .09091652 .09091632 .09091611 .09091591 .09091571
.09091551 .09091532 .09091513 .09091494 .09091475 .09091456
.09091438 .09091420 .09091402 .09091384 .09091367 .09091350
.09091333 .09091316 .09091299 .09091283 .09091267 .09091251
.09091235 .09091220 .09091204 .09091189 .09091175 .09091160
.09091145 .09091131 .09091117 .09091103 .09091090 .09091076
.09091063 .09091050 .09091037 .09091025 .09091012 .09091000
.09090988 .09090976 .09090964 .09090953 .09090942 .09090931
.09090920 .09090909 .09090899 .09090888 .09090878 .09090868
.09090858 .09090849 .09090839 .09090830 .09090821 .09090812
.09090804 .09090795 .09090787 .09090779 .09090771 .09090763
.09090755 .09090748 .09090740 .09090733 .09090726 .09090719
.09090713 .09090706 .09090700 .09090694 .09090688 .09090682
.09090676 .09090671 .09090666 .09090661 .09090656 .09090651
.09090646 .09090642 .09090637 .09090633 .09090629 .09090625
.09090621 .09090618 .09090614 .09090611 .09090608 .09090605
.09090602 .09090599 .09090597 .09090594 .09090592 .09090590
.09090588 .09090586 .09090585 .09090583 .09090582 .09090581
.09090579 .09090579 .09090578 .09090577 .09090577 .09090576
.09090576 .09090576 .09090576 .09090576 .09090576 .09090577
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```
..JOB*SLAZAK AND MUSORRAFITI       BOX  71    BOHR S
      PROGRAM THESIS
     0DIMENSION Y1(600),Y2(674),Y3(674),Y4(674),R(674),R1(6
     174),CE(674),A(674),Y6(674),Y7(674),F1(1),F2(1),F3(1),
     2F4(1),F5(1),F6(1),F7(1),F8(1),F9(1),F10(1),F11(1),F12
     3(1),F13(1),F14(1),F15(1),X(600),ITITLE(10),R2(667)
      DO 1234  I=1,10
 1234 ITITLE(I)=(8H        )
      ITITLE(1)=(8H SLAZAK )
      ITITLE(2)=(8HAND MUSO)
      ITITLE(3)=(8HRRAFITI )
      ITITLE(4)=(8HBOX 71  )
      ITITLE(5)=(8H  GOLD  )
      DO 999 I=1,600
  999 X(I)=I
      Z=79.
      PRINT 60
   600FORMAT(10H1        N 20H     BOHR RADII     20H      RYDBERGS
     1 20H      RYDBERGS      20H       RYDBERGS       24H COHESIVE KCAL P
     2ER MOLE  //// )
      HION=.666
      EASY=.500
      SY=.875
      SX=.0826
    2 ST=1.429
    9 DO 604  J=1,300
      ZN=J
      H=.01
      AK=ZN*H
     0SU=(1./LOGF(3.))*(LOGF(LOGF((1.-SX)*COSF(3.*SY)/(.021-SX)) )
     1-LOGF(ST))
      A(J)=(1.-SX)*COSF(SY*AK)/EXPF(ST*AK**SU)+SX
  604 CONTINUE
      DO 605  J=301,600
      ZN=J
      H=.01
      AK=ZN*H
      A(J)=.105/(AK+2.)
  605 CONTINUE
      H=.01
      B=2.*Z
      Q=2.*Z*(4.*(A(2)-1.)-2.*(A(3)-1.))/2.*H -2.*EASY
      R=2.*Z*(A(3)-2.*A(2)+1.)/(2.*H*H)
      F1=-B/2.
      F2=-B*F1/2. -Q/6.
      F3=-(B*F2-Q*F1-R)/12.
      F4=-(B*F3 -Q*F2 -R*F1)/20.
```

```
      F5=-(B *F4 -Q *F3 -R *F2)/30.
      F6=-(B*F5 -Q*F4 -R*F3)/42.
      F7=-(B*F6 -Q*F5-R*F4)/56.
      F8=-(B*F7-Q*F6 -R*F5)/72.
      F9=-(B*F8 -Q*F7-R*F6)/90.
      F10=-(B*F9-Q*F8-R*F7)/110.
      H=.01
      SK=2.*H
     0Y1(1)=H+F1*H*H +F2*H**3 +F3*H**4+F4*H**5 +F5*H**6
     1+F6*H**7+F7*H**8+F8*H**9 + F9*H**10+F10*H**11
     0Y1(2)=SK+F1*SK**2+F2*SK**3 + F3*SK**4+F4*SK**5
     1+F5*SK**6+F6*SK**7+F7*SK**8 +F8*SK**9+F9*SK**10
     2+F10*SK**11
      Y1(3)=Y1(2)*(2.-H*H*2.*(Z*A(2)/(H*2.)-EASY))-Y1(1)
      Y1(4)=Y1(3)*(2.-H*H*2.*(Z*A(3)/(H*3.)-EASY))-Y1(2)
      Y1(5)=Y1(4)*(2.-H*H*2.*(Z*A(4)/(H*4.)-EASY))-Y1(3)
      Y1(6)=Y1(5)*(2.-H*H*2.*(Z*A(5)/(H*5.)-EASY))-Y1(4)
      DO 12 I=2,599
      I1=I+1
      I6=I-1
      BO=I
      ON=I1
      Y1(I1)= Y1(I)*(2.-H*H*2.*(Z*A(I)/(H*BO)-EASY))-Y1(I6)
   12 CONTINUE
      K11=595
      DO 30 J=6,K11
      J1=J+1
      BO=J
      J6=J-1
      ON=J1
      J2=J+2
      J3=J+3
      J4=J+4
      J5=J+5
      J11=J-1
      J22=J-2
      J33=J-3
      HJ=J1
      HAL3=(Y1(J2)- Y1(J))*4./(5.*H)-(Y1(J3)-Y1(J11))/(5.*H)
     0HAL4=(Y1(J4)- Y1(J22))*4./(105.*H)-(Y1(J5)-Y1(J33))/
     1(280.*H)
      Y2(J1)=HAL3+HAL4
      Y3(J1)=Y1(J1)/(H*ON)
      Y4(J1)=Y3(J1)-Y2(J1)
      AB=ABSF(Y4(J1)      )
      IF(AB-1.E-3)13,13,30
   13 R(J1)=-2.*EASY+2.2/((H*ON)*(H*ON))
```

```
      R1(J1)=R(J1)+HION
      R2(J1)=2.*EASY
      CE(J1)=R1(J1)*310.5
      PRINT 221,J1,R2(J1),R(J1),Y4(J1),CE(J1)
  221 FORMAT(I10,1P5E20.8)
   30 CONTINUE
      EASY=EASY+.005
      IF(EASY-.600)2,2,556
  556 END
      END
```

```
..JOB*SLAZAK AND MUSORRAFITI        BOX  71                  SEARCH
     PROGRAM THESIS
    0DIMENSION Y1(830),Y2(83C),Y3(674),Y4(830),R(674),R1(674),CE(674),
    1A(830),Y6(674),Y7(674),F1(1),F2(1),F3(1),F4(1),F5(1),F6(1),
    2F7(1),F8(1),F9(1),F10(1),F11(1),F12(1),F13(1),F14(1),F15(1),
    3 R2(667),0(830),00(830)
     DO 999 I=1,600
  999 X(I)=I
     PRINT 60
  600FORMAT(10HT        N 20H      BOHR RADII      20H       RYDBERGS
    1 20H       RYDBERGS       20H        RYDBERGS        24H COHESIVE KCAL P
    2ER MCLE  //// )
      Z=79.
      EASY=.333
    2 ST=1.250
    7 SX=.047
    3 SY=.875
      SB=3.0
      SZ=LOGF((COSF(SY*SB))*(1.-SX)/(3.5369/Z-SX))
      SU=LOGF(SZ/ST)/LCGF(3.0)
      SG=3.0
      SE=.021
      SB=20.0
      SU1=(SE/((SB+SG)*(SE-SX))-SY*TANF(SY*SG))*(1./SZ)
      SA=SG*SZ/(SG**SU1)
      SD=SA-ST
      PRINT 525,SU1,SA,SD
  525 FORMAT(1P3E20.8)
    9 DO 604 J=1,300
      ZN=J
      H=.01
      AK=ZN*H
      A(J)=(1.-SX)*COSF(SY*AK)/EXPF(ST*A<**SU)+SX
  604 CONTINUE
      DO 605 J=301,830
      TT  =(3.+SB)*SE/(AK+SB)
      TK=1./Z
      IF(TT-TK)811,811,812
  811 A(J)=TK
      GO TO 605
  812 A(J)=TT
  605 CONTINUE
      H=.01
      B=2.*Z
      Q=2.*Z*(4.*(A(2)-1.)-2.*(A(3)-1.))/2.*H -2.*EASY
      R=2.*Z*(A(3)-2.*A(2)+1.)/(2.*H*H)
      F1=-B/2.
```

```
      F2=-B*F1/2. -Q/6.
      F3=-(B*F2-Q*F1-R)/12.
      F4=-(B*F3 -Q*F2 -R*F1)/20.
      F5=-(B *F4 -Q *F3 -R *F2)/30.
      F6=-(B*F5 -Q*F4 -R*F3)/42.
      F7=-(B*F6 -Q*F5-R*F4)/56.
      F8=-(B*F7-Q*F6 -R*F5)/72.
      F9=-(B*F8 -Q*F7-R*F6)/90.
      F10=-(B*F9-Q*F8-R*F7)/110.
      H=.01
      SK=2.*H
     0Y1(1)=H+F1*H*H +F2*H**3 +F3*H**4+F4*H**5 +F5*H**6
     1+F6*H**7+F7*H**8+F8*H**9 + F9*H** 10+F10*H**11
     0Y1(2)=SK+F1*SK**2+F2*SK**3 + F3*SK**4+F4*SK**5
     1+F5*SK**6+F6*SK**7+F7*SK**8 +F8*SK**9+F9*SK**10
     2+F10*SK**11
      DO 12 I=2,829
      I1=I+1
      I6=I-1
      BO=I
      ON=I1
      Y1(I1)=Y1(I)*(2.-H*H*2.*(Z*A(I)/(H*BO)-EASY))-Y1(I6)
   12 CONTINUE
      AB=Y1(820)
      PRINT 557,AB
  557 FORMAT(1P6E20.8)
      PRINT 111,EASY,SY,SX,ST,SU
  111 FORMAT(1P5E20.8)
      IF(AB-1.E-3)23,223,223
   23 ST=ST+.005
      AQ=ABSF(SD)
      IF(ST-1.940)3,3,22
  223 IF(SD-1.E-3)224,323,242
  224 IF(AQ-1.E-3)323,323,225
  242 IF(AQ-1.E-3)323,323,22
  225 SX=SX-.001
      ST=ST-.025
      GO TO 3
  323 HION = .666
      EASY=.500
      K33=1
      H=.01
   52 DO 191 L=1,K33
      B=2.*Z
      Q=2.*Z*(4.*(A(2)-1.)-2.*(A(3)-1.))/2.*H -2.*EASY
      R=2.*Z*(A(3)-2.*A(2)+1.)/(2.*H*H)
      F1=-B/2.
```

```
      F2=-B*F1/2. -Q/6.
      F3=-(B*F2-Q*F1-R)/12.
      F4=-(B*F3 -Q*F2 -R*F1)/20.
      F5=-(B *F4 -Q *F3 -R *F2)/30.
      F6=-(B*F5 -Q*F4 -R*F3)/42.
      F7=-(B*F6 -Q*F5-R*F4)/56.
      F8=-(B*F7-Q*F6 -R*F5)/72.
      F9=-(B*F8 -Q*F7-R*F6)/90.
      F10=-(B*F9-Q*F8-R*F7)/110.
      H=.01
      SK=2.*H
     0Y1(1)=H+F1*H*H +F2*H**3 +F3*H**4+F4*H**5 +F5*H**6
     1+F6*H**7+F7*H**8+F8*H**9 + F9*H**10+F10*H**11
     0Y1(2)=SK+F1*SK**2+F2*SK**3 + F3*SK**4+F4*SK**5
     1+F5*SK**6+F6*SK**7+F7*SK**8 +F8*SK**9+F9*SK**10
     2+F10*SK**11
      Y1(3)=Y1(2)*(2.-H*H*2.*(Z*A(2)/(H*2.)-EASY))-Y1(1)
      Y1(4)=Y1(3)*(2.-H*H*2.*(Z*A(3)/(H*3.)-EASY))-Y1(2)
      Y1(5)=Y1(4)*(2.-H*H*2.*(Z*A(4)/(H*4.)-EASY))-Y1(3)
      Y1(6)=Y1(5)*(2.-H*H*2.*(Z*A(5)/(H*5.)-EASY))-Y1(4)
      DO 42 I=2,599
      I1=I+1
      I6=I-1
      BO=I
      ON=I1
      Y1(I1)= Y1(I)*(2.-H*H*2.*(Z*A(I)/(H*BO)-EASY))-Y1(I6)
   42 CONTINUE
      K11=595
      DO 32 J=6,K11
      J1=J+1
      BO=J
      J6=J-1
      ON=J1
      J2=J+2
      J3=J+3
      J4=J+4
      J5=J+5
      J11=J-1
      J22=J-2
      J33=J-3
      HJ=J1
      HAL3=(Y1(J2)- Y1(J))*4./(5.*H)-(Y1(J3)-Y1(J11))/(5.*H)
      HAL4=(Y1(J4)- Y1(J22))*4./(105.*H)-(Y1(J5)-Y1(J33))/(280.*H)
      Y2(J1)=HAL3+HAL4
      Y3(J1)=Y1(J1)/(H*ON)
      Y4(J1)=Y3(J1)-Y2(J1)
      AB=ABSF(Y4(J1)     )
```

```
      IF(AB-1.E-3)13,13,32
  13  R(J1)=-2.*EASY+2.2/((H*CN)*(H*ON))
      R1(J1)=R(J1)+HION
      R2(J1)=2.*EASY
      CE(J1)=R1(J1)*310.5
      PRINT 221,J1,R2(J1),R(J1),Y4(J1),CE(J1)
 221  FORMAT(I10,1P5E20.8)
  32  CONTINUE
      EASY=EASY+.005
      IF(EASY-.75)52,52,191
 191  GO TO 556
  22  SX=SX+.001
      ST=ST-.025
      IF(SX-.095)3,3,556
 556  END
      END
```

```
..JOB*MUSORRAFITI AND SLAZAK           BJX 71    FERMI-GOLD
      PROGRAM THESIS
C     THOMAS-FERMI, HARTREE AND HARTREE-FOCH POTENTIALS
C     WERE USED IN LIKE   PROGRAMS TO MAKE SIMILIAR
C     CALCULATIONS AND THE VALUES OBTAINED COMPARED WITH
C     THOSE OBTAINED FROM THE SLAZAK-MUSORRAFITI POTENTIAL.
     ODIMENSION Y1(830),Y2(674),Y3(674),Y4(674),R(674),
     1R1(674),CE(674),A(830),Y6(674),Y7(674),X(830),ITITLE(
     210),R2(674)
      DO 1234  I=1,10
 1234 ITITLE(I)=(8H        )
      ITITLE(1)=(8H SLAZAK )
      ITITLE(2)=(8HAND MUSO)
      ITITLE(3)=(8HRRAFITI )
      ITITLE(4)=(8HBOX 71  )
      ITITLE(5)=(8HFERMI           )
      ITITLE(6)=(8HGOLD           )
      READ 223,(A(I),I=1,610)
      DO 998 I=611,830
  998 A(I)=A(610)
  223 FORMAT(5F10.0)
      DO 999 I=1,830
  999 X(I)=I
      CALL GRAPH2(830,X,A ,8,0,0,ITITLE,0,0,0,0,0,0,0,0)
      Z=79.
      HICN=.280
      EASY=.18
    2 H=.01
      B=2.*Z
      Q=2.*Z*(4.*(A(2)-1.)-2.*(A(3)-1.))/2.*H -2.*EASY
      R=2.*Z*(A(3)-2.*A(2)+1.)/(2.*H*H)
      F1=-B/2.
      F2=-B*F1/2. -Q/6.
      F3=-(B*F2-Q*F1-R)/12.
      F4=-(B*F3 -Q*F2 -R*F1)/20.
      F5=-(B *F4 -Q *F3 -R *F2)/30.
      F6=-(B*F5 -Q*F4 -R*F3)/42.
      F7=-(B*F6 -Q*F5-R*F4)/56.
      F8=-(B*F7-Q*F6 -R*F5)/72.
      F9=-(B*F8 -Q*F7-R*F6)/90.
      F10=-(B*F9-Q*F8-R*F7)/110.
      H=.01
      SK=2.*H
     0Y1(1)=H+F1*H**2+F2*H**3+F3*H**4+F4*H**5+F5*H**6
     1+F6*H**7+F7*H**8+F8*H**9+F9*H**10+F10*H**11
     0Y1(2)=SK+F1*SK**2+F2*SK**3 + F3*SK**4+F4*SK**5
     1+F5*SK**6+F6*SK**7+F7*SK**8 +F8*SK**9+F9*SK**10
```

```
     2+F10*SK**11
      Y1(3)=Y1(2)*(2.-H*H*2.*(Z*A(2)/(H*2.)-EASY))-Y1(1)
      Y1(4)=Y1(3)*(2.-H*H*2.*(Z*A(3)/(H*3.)-EASY))-Y1(2)
      Y1(5)=Y1(4)*(2.-H*H*2.*(Z*A(4)/(H*4.)-EASY))-Y1(3)
      Y1(6)=Y1(5)*(2.-H*H*2.*(Z*A(5)/(H*5.)-EASY))-Y1(4)
      DO 12 I=2,829
      I1=I+1
      I6=I-1
      BO=I
      ON=I1
      Y1(I1)= Y1(I)*(2.-H*H*2.*(Z*A(I)/(H*BO)-EASY))-Y1(I6)
   12 CONTINUE
      CALL GRAPH2(830,X,Y1,8,C,0,ITITLE,0,C,0,0,0,0,0,0)
      EASY=EASY+.01
      IF(EASY-.22)2,2,556
  556 END
      END
.9542       .8920       .8400       .8000       .7620
.7290       .6990       .6668       .6400       .6180
.5950       .5730       .5520       .5320       .5140
.4980       .4800       .4665       .4500       .4350
.4200       .4090       .3980       .3870       .3754
.3660       .3550       .3450       .3360       .3260
.3160       .3090       .300        .2920       .2860
.2790       .2720       .2660       .2600       .2525
.2470       .2420       .236        .2315       .226
.220        .216        .211        .206        .2015
.1975       .1928       .1887       .1850       .1810
.1775       .1742       .1708       .1670       .1638
.1605       .1575       .1545       .1518       .1490
.1463       .1443       .1410       .1385       .1360
.1338       .1315       .1292       .1275       .1250
.1225       .1221       .1190       .1170       .1150
.1135       .1119       .1100       .1082       .1067
.1051       .1035       .1018       .1000       .09823
.0972       .0950       .0934       .0918       .0901
.0882       .0867       .0852       .0838       .08258
.0814       .0802       .0791       .0780       .0770
.0759       .0749       .0739       .0729       .0718
.0709       .06995      .0690       .0681       .0672
.0664       .0655       .0647       .0639       .0631
.0625       .0617       .0609       .0601       .0594
.0587       .0580       .05730      .05665      .0560
.0554       .0548       .0542       .0536       .0530
.0524       .0518       .0512       .0506       .05005
.0495       .04895      .0484       .0479       .04739
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.0468      .04635     .0458      .0453      .0448
.0442      .04361     .0431      .0426      .0421
.0416      .04105     .04055     .0400      .0395
.0391      .0387      .03825     .0378      .03745
.0370      .03658     .0361      .0357      .03525
.03485     .03441     .03402     .03365     .03335
.03295     .03259     .03221     .0319      .03155
.0311      .0309      .0306      .0303      .0300
.0297      .0294      .0291      .0288      .0285
.02825     .02799     .02775     .02748     .02721
.0270      .0268      .0256      .0263      .0260
.02575     .02526     .02495     .02465     .0244
.02418     .02396     .02375     .02355     .02332
.02312     .02292     .02273     .02252     .0235
.02217     .0220      .0218      .02165     .02148
.02132     .02114     .02096     .02079     .02062
.02044     .02026     .02009     .01992     .01975
.01957     .01939     .01922     .01905     .01887
.01870     .01852     .01835     .01817     .01800
.01785     .01772     .01759     .01744     .01730
.01717     .01704     .01690     .01680     .01669
.01657     .01645     .01636     .01627     .01620
.01613     .01605     .01598     .01590     .01584
.01575     .01568     .01562     .01554     .01547
.01540     .01534     .01527     .01521     .015165
.015125    .015085    .015041    .015000    .01496
.01492     .01485     .01480     .014760    .014729
.014703    .014695    .014660    .014620    .014580
.014545    .014506    .014475    .014441    .014403
.014372    .014342    .014310    .014284    .014250
.014220    .014190    .014165    .014148    .014121
.014085    .014061    .014039    .014010    .013980
.013960    .013940    .013910    .013890    .013870
.013850    .013838    .013808    .013795    .013778
.013750    .013738    .013720    .013700    .013697
.013662    .013650    .013630    .013612    .013600
.013582    .013570    .013553    .013539    .013522
.013505    .013498    .013482    .013470    .013458
.013442    .013438    .013421    .013410    .013402
.013390    .013380    .013365    .013350    .013341
.013335    .013320    .013310    .013295    .013290
.013272    .013263    .013252    .013242    .013238
.013224    .013218    .013208    .013200    .013198
.013180    .013174    .013168    .013162    .013158
.013148    .013140    .013136    .013124    .013119
.013110    .013102    .013098    .013090    .013082
.013079    .013070    .013062    .013059    .013054
```

```
.013050    .013047    .013041    .013037    .013032
.013027    .013021    .013017    .013011    .013006
.013002    .0129970   .0129900   .0129860   .0129810
.0129758   .0129700   .0129642   .0129590   .012954
.012951    .012946    .012940    .012935    .012931
.012926    .012921    .012916    .012911    .012906
.012900    .0128970   .012892    .012887    .012883
.012878    .012874    .012870    .012865    .012861
.012857    .012853    .012849    .012845    .012841
.012837    .012832    .012828    .012824    .012821
.012817    .012813    .012809    .012806    .012801
.012797    .012795    .012791    .012787    .012783
.012779    .012776    .012773    .012770    .012767
.012764    .012760    .012758    .0127558   .012753
.012750    .012747    .012745    .012743    .012740
.012738    .012736    .012734    .012732    .012730
.0127275   .0127258   .0127240   .012722    .012720
.012719    .012717    .012716    .012715    .012714
.0127125   .012711    .012710    .012709    .0127078
.0127070   .0127060   .0127050   .0127040   .0127030
.0127020   .0127010   .0127000   .0126990   .0126980
.0126976   .0126968   .0126960   .0126952   .0126942
.0126938   .0126930   .0126922   .0126920   .0126910
.0126900   .0126898   .0126890   .0126885   .0126880
.0126872   .0126868   .0126862   .0126859   .0126852
.0126844   .0126840   .0126838   .0126830   .0126822
.0126820   .0126818   .0126810   .0126802   .0126799
.0126792   .0126790   .0126780   .0126776   .0126770
.0126772   .0126762   .0126760   .0126756   .0126750
.0126742   .0126740   .0126738   .0126730   .0126726
.0126720   .0126718   .0126712   .0126708   .0126700
.0126699   .0126692   .0126690   .0126685   .0126681
.0126679   .0126676   .0126672   .0126670   .0126668
.0126662   .0126660   .0126659   .0126656   .0126652
.0126650   .0126649   .0126648   .0126646   .0126645
.0126644   .0126642   .0126641   .0126640   .0126639
.0126638   .0126637   .0126636   .0126635   .0126634
.0126633   .0126632   .0126631   .0126630   .0126629
.01266285  .01266280  .01266275  .01266270  .01266265
.01266260  .01266255  .01266250  .01266245  .01266240
.01266235  .01266230  .01266225  .01266220  .01266215
.01266210  .01266205  .01266200  .01266195  .01266190
.01266185  .01266180  .01266175  .01266170  .01266165
.01266160  .01266155  .01266150  .01266145  .01266140
.01266135  .01266130  .01266125  .01266120  .01266115
.01266110  .01266105  .01266100  .01266095  .01266090
```

```
..JOB*SLAZAK AND MUSORRAFITI            GJLD
      PROGRAM THESIS
     0DIMENSION Y1(830),Y2(83C),Y3(674),Y4(830),R(674),
     1R1(674),CE(674),A(830),Y6(674),Y7(574),R2(667),X(830),
     2PSI(830),PSI2(830),PSIA(80C),PSI2A(800),X1(800),
     3ITITLE(10)
      DO 1234  I=1,10
 1234 ITITLE(I)=(8H        )
      ITITLE(1)=(8H SLAZAK )
      ITITLE(2)=(8HAND MUSO)
      ITITLE(3)=(8HRRAFITI )
      ITITLE(4)=(8HBCX 71  )
      ITITLE(5)=(8HOUR     )
      ITITLE(6)=(8HGOLD          )
      Z=79.
    2 ST=1.429
      EASY=.597
    7 SX=.0826
      SG=2.99
      SE=.020
      K=299
      K1=K+1
    3 SY=.875
      SB=(6.5-Z*SE*SG)/(Z*SE-1.)
      SU=.524676
    9 DO 604 J=1,K
      ZN=J
      H=.01
      AK=ZN*H
      A(J)=(1.-SX)*COSF(SY*AK)/EXPF(ST*AK**SU)+SX
  604 CONTINUE
      DO 605 J=K1,830
      ZN=J
      H=.01
      AK=ZN*H
      TT=(SG+SB)*SE/(AK+SB)
      TK=1./Z
      IF(TT-TK)811,811,812
  811 A(J)=TK
      GO TO 605
  812 A(J)=TT
  605 CONTINUE
   13 H=.01
      B=2.*Z
      Q=2.*Z*(4.*(A(2)-1.)-2.*(A(3)-1.))/2.*H -2.*EASY
      R=2.*Z*(A(3)-2.*A(2)+1.)/(2.*H*H)
      F1=-B/2.
```

```
      F2=-B*F1/2. -Q/6.
      F3=-(B*F2-Q*F1-R)/12.
      F4=-(B*F3 -Q*F2 -R*F1)/20.
      F5=-(B *F4 -Q *F3 -R *F2)/30.
      F6=-(B*F5 -Q*F4 -R*F3)/42.
      F7=-(B*F6 -Q*F5-R*F4)/56.
      F8=-(B*F7-Q*F6 -R*F5)/72.
      F9=-(B*F8 -Q*F7-R*F6)/90.
      F10=-(B*F9-Q*F8-R*F7)/110.
      H=.01
      SK=2.*H
     0Y1(1)=H+F1*H*H +F2*H**3 +F3*H**4+F4*H**5 +F5*H**6
     1+F6*H**7+F7*H**8+F8*H**9 + F9*H** 10+F10*H**11
     0Y1(2)=SK+F1*SK**2+F2*SK**3 + F3*SK**4+F4*SK**5
     1+F5*SK**6+F6*SK**7+F7*SK**8 +F8*SK**9+F9*SK**10
     2+F10*SK**11
      DO 12 I=2,829
      I1=I+1
      I6=I-1
      BO=I
      ON=I1
      Y1(I1)=Y1(I)*(2.-H*H*2.*(Z*A(I)/(H*BO)-EASY))-Y1(I6)
   12 CONTINUE
      DO 998 I=1,830
      X(I)=I
      H=.01
      ZN=I
      AK=ZN*H
      PSI(I)=Y1(I)/AK
      PSI2(I)=PSI(I)*PSI(I)
  998 CONTINUE
      N=1
      DO 901 I=30,830
      PSIA(N)=PSI(I)
      PSI2A(N)=PSI2(I)
      X1(N)=X(I)
      N=N+1
  901 CONTINUE
  556 END
      END
```

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Calculation of the lowest energy state o
3 2768 002 01148 8
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